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ERROR CONTROL FOR THE FEM APPROXIMATION OF AN UPSCALED THERMO-DIFFUSION SYSTEM WITH SMOLUCHOWSKI INTERACTIONS

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Abstract. We analyze a coupled system of evolution equations that describes the effect of thermal gradients on the motion and deposition of N populations of colloidal species diffusing and interacting together through Smoluchowski production terms. This class of systems is particularly useful in studying drug delivery, contaminant transport in complex media, as well as heat shocks thorough permeable media. The particularity lies in the modeling of the nonlinear and nonlocal coupling between diffusion and thermal conduction. We investigate the semidiscrete as well as the fully discrete *a priori* error analysis of the finite elements approximation of the weak solution to a thermo-diffusion reaction system posed in a macroscopic domain. The mathematical techniques include energy-like estimates and compactness arguments.

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1. Introduction

We are interested in quantifying the effect of coupled macroscopic fluxes[1] on the aggregation, fragmentation and deposition of large populations of colloids traveling through a porous medium. To do so, we are using a well-posed partly-dissipative coupled system of quasilinear parabolic equations posed in a connected open set Ω with sufficiently smooth boundary. The particular structure of the system has been obtained via periodic homogenization techniques in [2] [see e.g. Ref. [3] for a methodological upscaling procedure of reactive flows through arrays of periodic microstructures].

The primary motivation of this paper is to develop and analyze appropriate numerical schemes to compute at macroscopic scales approximate solutions to our thermo-diffusion system with Smoluchowski interactions. Accounting for the interplay between heat, diffusion, attraction-repulsion, and deposition of the colloidal particles is of paramount importance for a number of applications including the dynamics of the colloidal suspension in natural or man-made products (e.g. milk, paints, toothpaste) [4], drug-delivery systems [5], hierarchical assembly of biological tissues [6], group formation in actively interacting populations [7], or heat stocks in porous materials [8]. Further details on colloids and their practical relevance are given in [9, 10], e.g.

The discretizations shown in this paper have been successfully used in [11] to capture the effect of multiscale aggregation and deposition mechanisms on the colloids dynamics traveling within a saturated porous medium in the absence of thermal effects. Now, we are preparing the stage to include the Soret and Dufour transport contributions – cross-effects between diffusion and heat conduction; for more details on the macroscopic modeling of thermo-diffusion, we refer the reader to the monograph by De Groot and Mazur [1]. The *a priori* estimates are obtained in a similar fashion as for problems involving reactive flow in porous media (see, for instance, [12, 13] and references cited therein), however specifics of the cross transport, interaction terms, and of the non-dissipative (ode) structure play here an important role and need to be treated carefully. For the numerical analysis of case studies in cross diffusion, we refer the reader for instance to [14, 15] and [16]. Note that there is not yet a unified mathematical approach to deal with general cross-diffusion or thermo-diffusion systems. Due to the presence of the nonlinearly coupled transport terms, essential difficulties arise in controlling the temperature gradients (and the gradients in the concentrations of colloidal populations) especially in more space dimensions (see e.g. [17]), the problem sharing many common features with the Stefan-Maxwell system for multicomponent mixtures (compare Refs. [18, 19, 20] and the literature mentioned therein).

In this paper, we investigate the semidiscrete as well as the fully discrete *a priori* error analysis of the finite elements approximation of the weak solution to a thermo-diffusion reaction system posed in a macroscopic domain that allows for aggregation, dissolution as well as deposition of colloidal species. The main results are summarized in Theorem 4.7 and Theorem 5.2. The mathematical techniques used in the proofs include energy-like estimates and compactness arguments, exploiting the structure of the nonlocal coupling. Once these *a priori* estimates are proven and corrector estimates for the homogenization process explained in [2] become available, then the next natural analysis step is to prepare

[1]In this context, the fluxes are driven by a suitable combination of heat and diffusion gradients [1].

a functional framework for the design optimally convergent MsFEM schemes approximating, very much in the spirit of [21, 22], multiscale formulations of our thermo-diffusion system.

The paper has the following structure: Section 2 presents the setting of the model equations and briefly summarizes the meaning of the parameters and model components. We anticipate already at this point the main results. In Section 3, we list the main mathematical analysis aspects of our choice of thermo-diffusion system and briefly recall a collection of approximation theory results that are used in the sequel. Section 4 and Section 5 constitute the bulk of the paper. This is the place where we give the details of the proof of the semidiscrete and fully discrete *a priori* error control, i.e. the proofs for Theorem 4.7 and Theorem 5.2.

2. Formulation of the problem. Main results

Let I denote an open sub-interval within the time interval $(0,T]$, and let $x \in \Omega$ be the variable pointing out the space position. The unknowns of the system are the temperature field θ, the mobile colloidal populations u_i ($i \in \{1,\dots,N\}$), and the immobile (already deposited) colloidal populations v_i ($i \in \{1,\dots,N\}$). $N \in \mathbb{N}$ represents the amount of the monomers in the largest colloidal species considered. All unknowns depend on both space and time variables $(x,t) \in \Omega \times I$.

Definition 1. *Given $\delta > 0$, we introduce the mollifier:*

$$J_\delta(s) := \begin{cases} Ce^{1/(|s|^2-\delta^2)} & \text{if } |s| < \delta, \\ 0 & \text{if } |s| \geq \delta, \end{cases} \tag{1}$$

where the constant $C > 0$ is selected such that

$$\int_{\mathbb{R}^d} J_\delta = 1,$$

see [23] for details.

Definition 2. *Using J_δ from (1), define the mollified gradient:*

$$\nabla^\delta f := \nabla \left[\int_{B(x,\delta)} J_\delta(x-y) f(y) dy \right], \tag{2}$$

where $B(x,\delta) \subset \mathbb{R}^d$ is a ball centered in $x \in \Omega$ with radius δ, $d \geq 1$.

With Definition 2 at hand, the following inequalities hold for all $f \in L^\infty(\Omega)$ and $g \in L^p(\Omega;\mathbb{R}^d)$ (with $1 \leq p \leq \infty$):

$$\|\nabla^\delta f \cdot g\|_{L^p(\Omega)} \leq C \|f\|_{L^\infty(\Omega)} \|g\|_{L^p(\Omega;\mathbb{R}^d)}, \tag{3}$$

$$\|\nabla^\delta f\|_{L^p(\Omega)} \leq C \|f\|_{L^2(\Omega)}, \tag{4}$$

where the constant C depends on the choice of the parameter δ and structure of the mollifier J_δ.

For all $t \in I$, the setting of our thermo-diffusion equations is the following: Find the triplet (θ, u_i, v_i) satisfying

$$\partial_t\theta + \nabla\cdot(-K\nabla\theta) - \sum_{i=1}^{N} T_i\nabla^\delta u_i\cdot\nabla\theta = 0 \qquad \text{in } \Omega, \tag{5}$$

$$\partial_t u_i + \nabla\cdot(-D_i\nabla u_i) - F_i\nabla^\delta\theta\cdot\nabla u_i + \tag{6}$$

$$+ A_i u_i - B_i v_i = R_i(u_i) \qquad \text{in } \Omega, \tag{7}$$

$$\partial_t v_i = A_i u_i - B_i v_i \qquad \text{in } \Omega, \tag{8}$$

$$- K\nabla\theta\cdot n = 0 \qquad \text{on } \partial\Omega, \tag{9}$$

$$u_i = 0 \qquad \text{on } \partial\Omega, \tag{10}$$

$$\theta(0,\cdot) = \theta^0(\cdot) \qquad \text{in } \Omega, \tag{11}$$

$$u_i(0,\cdot) = u_i^0(\cdot) \qquad \text{in } \Omega, \tag{12}$$

$$v_i(0,\cdot) = v_i^0(\cdot) \qquad \text{in } \Omega. \tag{13}$$

Here, we use the Smoluchowski population balance equation, originally proposed in [24], to account for the production terms $R_i(u)$:

We want to model the transport of aggregating colloidal particles under the influence of thermal gradients. We use to account for colloidal aggregation:

$$R_i(u) := \frac{1}{2}\sum_{k+j=i}\beta_{kj}u_k u_j - \sum_{j=1}^{N}\beta_{ij}u_i u_j, \qquad i > 1$$

Colloidal aggregation rates β_{ij} are described in more detail in [10]. Here, it's enough for us that they are positive and bounded.

Here for all $i \in \{1,\dots,N\}$, the parameters K, D_i, F_i and T_i are effective transport coefficients for heat conduction, colloidal diffusion as well as Soret and Dufour effects. Furthermore, A_i and B_i are effective deposition coefficients. θ^0 is the initial temperature profile, while u_i^0 and v_i^0 are the initial concentrations of colloids in mobile, and respectively, immobile state. General motivation on the ingredients of this system (particularly on Soret and Dufour effects) can be found in [1]. Note that as direct consequence of fixing the threshold N, the system coagulates colloidal species (groups) until size N only.

This particular structure of the system has been derived in [2] by means of periodic homogenization arguments (two-scale convergence), scaling up the involved physicochemical processes from the pore scale (microscopic level, representative elementary volume (REV)) to a macroscopically observable scale.

Remark 2.1. *Theorem 4.4 in [2] ensures the weak solvability of the system (5)–(13). Furthermore, under mild assumptions on the data and the parameters the weak solution is positive a.e. and satisfies a weak maximum principle. The basic properties of the weak solutions to (5)–(13) are given in Section 3.*

Denoting by $\theta^h(t)$ the continuous-in-time and semidiscrete-in-space approximation of $\theta(t)$ and by $\theta^{h,n}$ the corresponding fully discrete approximation, with similar notation for the other unknowns, and taking all norms to mean L_2 unless explicitly specified otherwise, we can formulate our main result: For all $t, t_n \in I$, the following *a priori* estimates hold:

$$\|\theta^h(t) - \theta(t)\| + \sum_{i=1}^{N} \|u_i^h(t) - u_i(t)\| + \sum_{i=1}^{N} \|v_i^h(t) - v_i(t)\|$$
$$\leq C_1\|\theta^{0,h} - \theta^0\| + C_2(\|u_i^{0,h} - u_i^0\| + \|v_i^{0,h} - v_i^0\|) + C_3h^2 \tag{14}$$

and

$$\|\theta^{h,n} - \theta^n\| + \sum_{i=1}^{N} \|u_i^{h,n} - u_i^n\| + \sum_{i=1}^{N} \|v_i^{h,n} - v_i^n\|$$
$$\leq C_4\|\theta^{h,0} - \theta^0\| + C_5 \left(\sum_{i=1}^{N} \|u_i^{h,0} - u_i^0\| + \sum_{i=1}^{N} \|v_i^{h,0} - v_i^0\|\right)$$
$$+ C_6(h^2 + \tau). \tag{15}$$

The constants $C_1, \ldots, C_6$ depend on data, but are independent of the grid parameters h and τ. The hypotheses and the results under which (14) and (15) hold are stated in Theorem 4.7 and Theorem 5.2, respectively.

The following Sections focus exclusively on the proof of these inequalities.

3. Concept of weak solution. Technical preliminaries. Available results.

Our concept of weak solution is detailed as follows:

Definition 3. *The triplet (θ, u_i, v_i) is a solution to (5)-(13) if the following holds:*

$$\begin{aligned} &\theta, u_i \in H^1(0,T; L^2(\Omega)) \cap L^\infty(0,T; H^1(\Omega)), \\ &v_i \in H^1(0,T; L^2(\Omega)), \end{aligned} \tag{16}$$

and for all $t \in J$ and $\phi \in H^1(\Omega)$:

$$(\partial_t\theta, \phi) + (K\nabla\theta, \nabla\phi) - \sum_{i=1}^{N}(T_i\nabla^\delta u_i \cdot \nabla\theta, \phi) = 0, \tag{17}$$

$$(\partial_t u_i, \phi) + (D_i\nabla u_i, \nabla\phi) - (F_i\nabla^\delta\theta \cdot \nabla u_i, \phi)$$
$$+ (A_iu_i - B_iv_i, \phi) = (R_i(u), \phi), \tag{18}$$

$$(\partial_t v_i, \phi) = (A_iu_i - B_iv_i, \phi). \tag{19}$$

To be able to ensure the solvability of our thermo-diffusion problem, we assume that the following set of assumptions on the data, i.e. (A_1)-(A_2) hold true:

- **(A_1):** T_i, F_i, A_i, B_i are positive constants for $i \in \{1, \ldots, N\}$, and there exist m and M such that: $0 < m \leq K \leq M$ and $0 < m \leq D_i \leq M$.
- **(A_2):** $\theta^0 \in L^\infty_+(\Omega) \cap H^2(\Omega), u_i^0 \in L^\infty_+(\Omega) \cap H^2(\Omega), v_i^0 \in L^\infty_+(\Gamma)$ for $i \in \{1, \ldots, N\}$.

Fix $h > 0$ sufficiently small and let T_h be a triangulation of Ω with

$$\max_{\tau\in \mathrm{T}_h} diam(\tau) \leq h.$$

Let S_h denote the finite dimensional space of continuous functions on Ω that reduce to linear functions in each of the triangles of T_h and vanish on $\partial\Omega$. Let $\{P_j\}_{j=1}^{N_h}$ be the interior vertices of T_h with $N_h \in \mathbb{N}$. A function in S_h is then uniquely determined by its values at the points P_j. Let Φ_j be the pyramid function in S_h which takes value 1 at P_j, but vanishes at the other vertices. Then $\{\Phi_j\}_{j=1}^{N_h}$ forms a basis for S_h. Consequently, every φ in S_h can be uniquely represented as

$$\varphi(x) = \sum_{j=1}^{N_h} \alpha_j \Phi_j(x), \quad \text{with } \alpha_j := \Phi(P_j), j \in \{1, \dots, N_h\}, \tag{20}$$

see e.g. Ref. [25].

A smooth function σ defined on Ω which vanishes on $\partial\Omega$ can be approximated by its interpolant $I_h\sigma$ in S_h defined as:

$$I_h\sigma(x) := \sum_{j=1}^{N_h} \sigma(P_j)\Phi_j(x). \tag{21}$$

We denote below by $\|\cdot\|$ the norm of the space $L_2(\Omega)$ and by $\|\cdot\|_s$ that in the Sobolev space $H^s(\Omega) = W_2^s(\Omega)$ with $s \in \mathbb{R}$. If $s = 0$ we suppress the index.

We recall that for functions v lying in $H_0^1(\Omega)$, the objects $\|\nabla v\|$ and $\|v\|_1$ are equivalent norms. Let us also recall Friedrichs' lemma (see, for instance, [26, 27]): there exist constants $c_F > 0$ and $C_F > 0$ (depending on Ω, see Ref. [28] for explicit expressions for these constants) such that

$$c_F\|\sigma\|_1 \le C_F\|\nabla\sigma\| \le \|\sigma\|_1, \quad \forall \sigma \in H_0^1(\Omega). \tag{22}$$

The following error estimates for the interpolant $I_h\sigma$ of σ [cf. (21)] are well-known (see, e.g., [26] or [27]), namely for all $\sigma \in H^2(\Omega) \cap H_0^1(\Omega)$ we have

$$\|I_h\sigma - \sigma\| \le Ch^2\|\sigma\|_2 \tag{23}$$

$$\|\nabla(I_h\sigma - \sigma)\| \le Ch\|\sigma\|_2. \tag{24}$$

Testing the equations (5)-(6) with $\varphi \in S_h$ leads to the following semi-discrete weak formulation of (5)-(13) as given in Definition 4.

Definition 4. *The triplet (θ^h, u_i^h, v_i^h) is a semidiscrete solution to (5)-(13) if the following identities hold true for all $t \in I$ and $\varphi \in S_h$:*

$$(\partial_t\theta^h, \varphi) + (K\nabla\theta^h, \nabla\varphi) - \sum_{i=1}^{N}(T_i\nabla^\delta u_i^h \cdot \nabla\theta^h, \varphi) = 0 \tag{25}$$

$$\begin{aligned}&(\partial_t u_i^h, \varphi) + (D_i\nabla u_i^h, \nabla\varphi) - (F_i\nabla^\delta\theta^h \cdot \nabla u_i^h, \varphi)\\ &\qquad + (A_i u_i^h - B_i v_i^h, \varphi) = (R_i(u^h), \varphi)\end{aligned} \tag{26}$$

$$(\partial_t v_i^h, \varphi) = (A_i u_i^h - B_i v_i^h, \varphi) \tag{27}$$

$$\theta^h(0) = \theta^{0,h} \tag{28}$$

$$u_i^h(0) = u_i^{0,h} \tag{29}$$

$$v_i^h(0) = v_i^{0,h}. \tag{30}$$

Here, $\theta^{0,h}$, $u_i^{0,h}$, and $v_i^{0,h}$ are suitable approximations of θ^0, u_i^0, and v_i^0 respectively in the finite dimensional space S_h.

Remark 3.1. *Note that v_i as a solution to (8) can be expressed as:*

$$v_i(t) = \left(\int_0^t A_i u_i(s) e^{B_i s} ds \right) e^{-B_i t} + v_i^0 e^{-B_i t} \qquad \text{for all } t \in I. \tag{31}$$

We will make this substitution later and also use (31) to obtain an error estimate for v_i^h based on the error estimate for u_i^h. This path can be followed due to the linearity of the equation. If the right-hand side of the ordinary differential equations becomes nonlinear, then a one-sided Lipschitz structure is needed to allow for the Gronwall argument to work.

Remark 3.2. *The existence of solutions in the sense of Definition 3 is ensured by periodic homogenization arguments in [2], while the existence of solutions in the sense of Definition 4 follows by standard arguments. We omit to show the details of the existence proofs. Note that the existence of the respective solutions is nevertheless re-obtained here by straightforward compactness arguments. The proof of uniqueness of both kinds of solutions follows the lines of [2].*

We represent the approximate solutions to the system (5)–(13) by means of the standard Galerkin Ansatz as:

$$u_i^h(x,t) := \sum_{j=1}^{N_h} \alpha_{ij}(t) \Phi_j(x),$$

$$\theta^h(x,t) := \sum_{j=1}^{N_h} \beta_j(t) \Phi_j(x),$$

$$v_i^h(x,t) := \sum_{j=1}^{N_h} \gamma_{ij}(t) \Phi_j(x)$$

for all $(x,t) \in \Omega \times I$. Based on the Galerkin projections, the semidiscrete model equations read:

$$\sum_{j=1}^{N_h} \beta'_{ij}(t)(\Phi_j, \Phi_k) + \sum_{j=1}^{N_h} \beta_{ij}(K_i \nabla \Phi_j, \nabla \Phi_k) - \sum_{i=1}^{N} T_i \sum_{j=1}^{N_h} \sum_{l=1}^{N_h} \beta_{ij}(t) \alpha_{il}(t)(\nabla^\delta \Phi_l \cdot \nabla \Phi_j, \Phi_k) = 0 \tag{32}$$

$$\sum_{j=1}^{N_h} \alpha'_{ij}(t)(\Phi_j, \Phi_k) + \sum_{j=1}^{N_h} \alpha_{ij}(D_i \nabla \Phi_j, \nabla \Phi_k) - F_i \sum_{j=1}^{N_h} \sum_{l=1}^{N_h} \alpha_{ij}(t) \beta_l(t)(\nabla^\delta \Phi_l \cdot \nabla \Phi_j, \Phi_k) = (R_i(\sum_{j=1}^{N_h} \alpha_{ij}(t) \Phi_j), \Phi_k). \tag{33}$$

To abbreviate the writing of (32)-(33), we define:

$$\begin{aligned}
&\alpha_i := \alpha_i(t) = (\alpha_{i1}(t), \ldots, \alpha_{i,N_h}(t))^T,\\
&\beta := \beta(t) = (\beta_1(t), \ldots, \beta_{N_h}(t))^T,\\
&\gamma_i := \gamma_i(t) = (\gamma_{i1}(t), \ldots, \gamma_{i,N_h}(t))^T,\\
&G := (g_{jk}),\ g_{jk} := (\Phi_j, \Phi_k),\\
&H_i^u := (h_{ijk}^u),\ h_{ijk}^u := (D_i \nabla \Phi_j, \nabla \Phi_k),\\
&H^\theta := (h_{jk}^\theta),\ h_{jk}^\theta := (K \nabla \Phi_j, \nabla \Phi_k),\\
&M := (m_{jkl}),\ m_{jkl} := (\nabla^\delta \Phi_l \cdot \Phi_j, \Phi_k).
\end{aligned}$$

Then (32)-(33) become:

$$\tag{34} \begin{cases}
G\beta' + H^\theta \beta - \sum_{i=1}^N T_i \alpha_i^T M \beta = 0\\
G\alpha_i' + H_i^u \alpha_i - F_i \beta^T M \alpha_i + G(A_i \alpha_i - B_i \gamma_i)\\
= (R_i(\sum_{j=1}^{N_h} \alpha \Phi_j), \Phi_k)\\
G\gamma_i' = A_i G \alpha_i - B_i G \gamma_i\\
\beta(0) = \beta^0\\
\alpha_i(0) = \alpha_i^0\\
\gamma_i(0) = \gamma_i^0.
\end{cases}$$

Note that (34) is a nonlinear system of coupled ordinary differential equations. Based on (A_1)–(A_2), we see not only that H^θ and H_i^u are positive definite, but also that the right-hand side of the differential equations form a global Lipschitz continuous function, fact which ensures the well-posedness of the Cauchy problem (34) on I and eventually on its continuation on the whole interval $(0, T]$; we refer the reader to [29] for this kind of extension arguments for ordinary differential equations. Essentially, we get a unique solution vector

$$(\beta, \alpha_i, \gamma_i) \in C^1(\bar{I})^{N^h} \times C^1(\bar{I})^{NN^h} \times C^1(\bar{I})^{NN^h}$$

satisfying (34); see [30] for the proof of the global Lipschitz property of the right-hand side of a similar system of ordinary differential equations.

4. Semi-discrete error analysis

Our goal is to estimate the a priori error between the weak solutions of (60)–(65) and the weak solutions of (5)–(13). We proceed very much in the spirit of Thomeé [31]; cf., for instance, Chapter 13 and Chapter 14.

We write the error as a sum of two terms:

$$\tag{35} \theta^h - \theta = (\theta^h - \tilde{\theta}^h) + (\tilde{\theta}^h - \theta) = \psi + \rho.$$

In (35), $\tilde{\theta}^h$ is the elliptic projection in S_h of the exact solution θ, i.e. $\tilde{\theta}^h$ satisfies for all $t \geq 0$:

$$\tag{36} (K\nabla(\tilde{\theta}^h(t) - \theta(t)), \nabla\varphi) - \sum_{i=1}^N (T_i \nabla^\delta u_i \cdot \nabla(\tilde{\theta}^h(t) - \theta(t)), \varphi) = 0$$

for all $\varphi \in S_h$.

Lemma 4.1. *Let $k \in C^1(\bar{\Omega})$, $b \in L^\infty(\Omega, \mathbb{R}^3)$, and $\nabla \cdot b \in L^\infty(\Omega)$. Suppose that $\gamma \in H_0^1(\Omega)$ is a weak solution to the elliptic boundary-value problem*

$$-\nabla \cdot (k\nabla\gamma + b\gamma) = \delta \quad \text{in } \Omega, \quad \gamma = 0 \quad \text{on } \partial\Omega. \tag{37}$$

Additionally, assume

$$\partial\Omega \in C^2. \tag{38}$$

Then we have

$$\|\gamma\|_2 \le C\|\delta\|. \tag{39}$$

Proof. The proof of this result is a particular case of the proof of Theorem 4 given in [23, p. 317]. We omit to repeat the arguments here. □

Remark 4.2. *The condition (38) can be relaxed to Ω being a convex polygon, see [32, p. 147] (compare Theorem 3.2.1.2 and Theorem 3.2.1.3).*

Lemma 4.3. *Let $k \in L^2(\Omega)$ and $b \in L^\infty(\Omega, \mathbb{R}^3)$, and $k(x) \ge m > 0$, and $m > \|b\|_\infty C_F$, where C_F is the constant entering (22). Suppose that $\gamma \in H_0^1(\Omega)$ is a weak solution of the elliptic boundary-value problem*

$$-\nabla \cdot (k\nabla\gamma + b\gamma) = \delta \quad \text{in } \Omega, \quad \gamma = 0 \quad \text{on } \partial\Omega. \tag{40}$$

Then we have

$$\|\gamma\|_2 \le C\|\delta\|. \tag{41}$$

Proof. We can directly verify that

$$\begin{aligned} m\|\gamma\|^2 &\le (k\nabla\gamma, \nabla\gamma) = (\delta, \gamma) + (b \cdot \gamma, \nabla\gamma) \\ &\le \|\delta\|\|\gamma\| + \|b\|_\infty \|\gamma\|\|\nabla\gamma\| \\ &\le \|\delta\|\|\gamma\| + \|b\|_\infty C_F \|\nabla\gamma\|^2. \end{aligned}$$

Here, we used the Friedrichs inequality (22). Since $m > \|b\|_\infty C_F$, we have (41). □

Lemma 4.4. *Take $k \in L^\infty(\Omega) \cap H^1(\Omega)$ and $b \in L^\infty(\Omega, \mathbb{R}^3) \cap H^1(\Omega, \mathbb{R}^3)$ and assume that there exist m and M such that $0 < m \le k(x) \le M$ for all $x \in \Omega$. Let $w \in H^2(\Omega) \cap H_0^1(\Omega)$ satisfying*

$$(k\nabla(w_h - w), \nabla\varphi) - (b \cdot \nabla(w_h - w), \varphi) = 0 \qquad \text{for all } \varphi \in S_h. \tag{42}$$

Then the following estimates hold:

$$\|\nabla(w_h - w)\| \le C_1 h \|w\|_2 \tag{43}$$

$$\|w_h - w\| \le C_0 h^2 \|w\|_2. \tag{44}$$

Here, the constant C_1 depends on T_h, m, and M. The constant C_0 depends additionally on the upper bound of ∇k and b in the corresponding L^∞-norm.

Proof. We proceed very much in the spirit of Ciarlet estimates. By (A_1), we have that

$$\begin{aligned} m\|\nabla(w_h - w)\|^2 &\le (k\nabla(w_h - w), \nabla(w_h - w)) = \\ &(k\nabla(w_h - w), \nabla(w_h - \varphi)) + (k\nabla(w_h - w), \nabla(\varphi - w)) = \\ &(b \cdot \nabla(w_h - w), w_h - \varphi) + (k\nabla(w_h - w), \nabla(\varphi - w)) \le \\ &\|b\|_\infty \|\nabla(w_h - w)\| \|w_h - \varphi\| + M\|\nabla(w_h - w)\| \|\nabla(\varphi - w)\| \end{aligned}$$

Take $\varphi := I_h w$ - the Clement interpolant of w. Then we have:

$$\begin{aligned} m\|\nabla(w_h - w)\| &\le \|b\|_\infty(\|w_h - w\| + \|I_h w - w\|) \\ &+ M\|\nabla(I_h w - w)\| \le C_1 h \|w\|_2, \end{aligned} \tag{45}$$

which yields

$$\begin{aligned} \|\nabla(w_h - w)\| &\le (C_1 h + C_2\|b\|_\infty h^2)\|w\|_2 \\ &+ \frac{\|b\|_\infty}{m}\|w_h - w\|. \end{aligned} \tag{46}$$

It is worth noting that (46) leads to (43) when we show later that (at least)

$$\|w_h - w\| \le Ch\|w\|_2.$$

Next, we show (44) using a duality argument. Let $\gamma \in H_0^1(\Omega)$ solve the problem

$$-\nabla \cdot (k\nabla\gamma - b\gamma) = \delta \quad \text{in } \Omega, \quad \gamma = 0 \quad \text{on } \partial\Omega.$$

Then

$$\begin{aligned} (w_h - w, \delta) &= (w_h - w, -\nabla \cdot (k\nabla\gamma - b\gamma)) \\ &= (k\nabla(w_h - w), \nabla\gamma) - (b \cdot \nabla(w_h - w), \gamma) \\ &= (k\nabla(w_h - w), \nabla(\gamma - \varphi)) - (b \cdot \nabla(w_h - w), \gamma - \varphi) \\ &+ (k\nabla(w_h - w), \nabla\varphi) - (b \cdot \nabla(w_h - w), \varphi). \end{aligned}$$

Let $\varphi := I_h\gamma$ and use (42):

$$\begin{aligned} (w_h - w, \delta) \le M\|\nabla(w_h - w)\| \|\nabla(\gamma - I_h\gamma)\| \\ + \|b\|_\infty \|\nabla(w_h - w)\| \|\gamma - I_h\gamma\|. \end{aligned}$$

Using the standard approximation properties for $I_h\gamma$, we get:

$$(w_h - w, \delta) \le (C_1 M h + C_2\|b\|_\infty h^2)\|\gamma\|_2 \|\nabla(w_h - w)\|. \tag{47}$$

Using $\delta := w_h - w$ in (47), and either Lemma 4.1 or Lemma 4.3, we obtain:

$$\|w_h - w\| \le (C_1 M h + C_2\|b\|_\infty h^2)C_3\|\nabla(w_h - w)\|. \tag{48}$$

Using (48) in (46) leads to:

$$\|\nabla(w_h - w)\| \le C_1 h\|w\|_2 + C_2 h\|\nabla(w_h - w)\|. \tag{49}$$

After solving the recurrence in (49), (43) is proven, and hence (44) follows from (48). □

Lemma 4.5. *Let $\tilde\theta^h$ be defined by (36), and let $\rho := \tilde\theta^h - \theta$. Then the following estimates hold:*

$$\|\rho(t)\| + h\|\nabla\rho(t)\| \le C(\theta)h^2 \qquad t \in I, \tag{50}$$

$$\|\rho_t(t)\| + h\|\nabla\rho_t(t)\| \le C(\theta)h^2 \qquad t \in I. \tag{51}$$

Proof. Using Lemma 4.4, we have that $\|\nabla\rho\| \leq C_1 h\|\theta\|_2$ and $\rho \leq C_0 h^2\|\theta\|_2$, so (50) follows by adding these estimates.

To obtain (51), we differentiate (36) with respect to time:

$$(k\nabla\rho_t, \nabla\varphi) - (b_t \cdot \nabla\rho + b \cdot \nabla\rho_t, \varphi) = 0$$

Assuming k uniformly bounded, which it is, since it doesn't depend on θ in our case:

$$\begin{aligned} m\|\nabla\rho_t\|^2 &\leq (k\nabla\rho_t, \nabla\rho_t) = (k\nabla\rho_t, \nabla(\tilde{\theta}^h_t - \varphi + \varphi - \theta_t)) \\ &= (k\nabla\rho_t, \nabla(\varphi - \theta_t)) + (k\nabla\rho_t, \nabla(\tilde{\theta}^h - \varphi)) \\ &= (k\nabla\rho_t, \nabla(\varphi - \theta_t)) + (b_t \cdot \nabla\rho + b \cdot \nabla\rho_t, \tilde{\theta}^h - \varphi) \end{aligned}$$

We have used (36) in the last equation since $(\tilde{\theta}^h - \varphi) \in S_h$. Thus we get that

$$m\|\nabla\rho_t\|^2 \leq M\|\nabla\rho_t\|\|\nabla(\varphi - \theta_t)\| + (C_1(b)\|\nabla\rho\| + C_2(b)\|\nabla\rho_t\|)\|\tilde{\theta}^h - \varphi\|$$

Now, take $\varphi := I_h\theta_t$ to obtain:

$$\begin{aligned} m\|\nabla\rho_t\| &\leq M\|\nabla\rho_t\|Ch\|\theta_t\|_2 + (C_1(b)\|\nabla\rho\| + C_2(b)\|\nabla\rho_t\|)(\|\rho_t\| + Ch\|\theta_t\|_2) \\ &\leq \frac{m}{2}\|\nabla\rho_t\|^2 + Ch^2\|\theta_t\|_2^2 + Ch(\|\rho_t\| + Ch\|\theta_t\|_2) \\ &\quad + C_2(u)\|\nabla\rho_t\|\|\rho_t\| + C_2(u)Ch\|\nabla\rho_t\|\|\theta_t\|_2. \end{aligned}$$

Using Young's inequality a few times, it finally follows that:

$$\|\nabla\rho_t\|^2 \leq C_1 h^2 + C_2\|\rho_t\|^2, \tag{52}$$

where C_1 and C_2 are independent of h.

Now, we use the duality argument as in Lemma 4.4 to gain:

$$\begin{aligned} (\rho_t, \delta) &= (\rho_t, -\nabla \cdot (k\nabla\gamma - b\gamma)) = (k\nabla\rho_t, \nabla\gamma) - (b \cdot \nabla\rho_t, \gamma) \\ &= (k\nabla\rho_t, \nabla(\gamma - \varphi)) - (b \cdot \nabla\rho_t, \gamma - \varphi) + (k \cdot \nabla\rho_t, \nabla\varphi) - (b \cdot \nabla\rho_t, \varphi) \\ &= (k\nabla\rho_t, \nabla(\gamma - \varphi)) - (b \cdot \nabla\rho_t, \gamma - \varphi). \end{aligned}$$

Choosing $\varphi := I_h\gamma$ and $\delta := \rho_t$ yields

$$\begin{aligned} \|\rho_t\|^2 &\leq C_1\|\nabla\rho_t\|(Mh + \|b\|_\infty h^2)\|\gamma\|_2 \\ &\leq C_2\|\nabla\rho_t\|(Mh + \|b\|_\infty h^2)\|\delta\| \leq \\ &\leq C_2\|\nabla\rho_t\|(Mh + \|b\|_\infty h^2)\|\rho_t\|. \end{aligned}$$

We now see that

$$\|\rho_t\| \leq C(u, \theta)h\|\nabla\rho_t\|. \tag{53}$$

Combining (52) and (53) leads to convenient recurrence relations, thus proving the statement of the Lemma. □

Lemma 4.6. *Let $\tilde{\theta}^h$ be defined by (36). Then:*

$$\|\nabla\tilde{\theta}^h(t)\|_\infty \leq C(\theta) \qquad t \in I. \tag{54}$$

Proof. We rely now on the inverse estimate:

$$\|\nabla\varphi\|_\infty \leq Ch^{-1}\|\nabla\varphi\| \qquad \forall\varphi \in S_h \tag{55}$$

The statement (55) is trivial to prove for linear approximation functions, since in this case $\nabla\varphi$ is constant on each triangle. Using Lemma 4.5 and the known error estimate for $I_h\theta$, we have:

$$\begin{aligned} \|\nabla(\tilde{\theta}^h - I_h\theta)\|_\infty &\leq Ch^{-1}\|\nabla(\tilde{\theta}^h - I_h\theta)\| \\ &\leq Ch^{-1}(\|\nabla\rho\| + \|\nabla(I_h\theta - \theta)\|) \leq C(\theta). \end{aligned} \tag{56}$$

□

The main result on the *a priori* error control for the semi-discrete FEM approximation to our original system is given in the next Theorem.

Theorem 4.7. *Let* (θ, u_i, v_i) *solve (16)-(19) and* (θ^h, u_i^h, v_i^h) *solve (60)-(65), and let assumptions* (A_1)*-*(A_2) *hold. Then the following inequalities hold:*

$$\|\theta^h(t) - \theta(t)\| \leq C\|\theta^{0,h} - \theta^0\| + C(\theta)h^2 \qquad t \in I, \tag{57}$$

$$\|u_i^h(t) - u_i(t)\| \leq C\|u_i^{0,h} - u_i^0\| + C(u_i)h^2 \qquad t \in I, i \in \{1, \ldots, N\}. \tag{58}$$

Proof. With an error splitting as in (35), it is enough to show a suitable upper bound for $\psi := \theta^h - \tilde{\theta}^h$. We proceed in the following manner:

$$\begin{aligned} (\partial_t\psi, \varphi) + (K\nabla\psi, \nabla\varphi) &= (\partial_t\theta^h, \varphi) + (K\nabla\theta^h, \nabla\varphi) - \sum_{i=1}^N (T_i\nabla^\delta u_i^h \cdot \theta^h, \varphi) \\ &+ \sum_{i=1}^N (T_i\nabla^\delta u_i^h \cdot \theta^h, \varphi) - (\partial_t\tilde{\theta}^h, \varphi) - (K\nabla\tilde{\theta}^h, \nabla\varphi) \\ &= -(\partial_t(\theta + \rho), \varphi) - (K\nabla(\theta + \rho), \nabla\varphi) + \sum_{i=1}^N (T_i\nabla^\delta u_i^h \cdot \theta^h, \varphi) \\ &= -(\partial_t\rho, \varphi) - (K\nabla\rho, \nabla\varphi) + \sum_{i=1}^N (T_i\nabla^\delta u_i \cdot \nabla\rho, \varphi) \\ &+ \sum_{i=1}^N (T_i(\nabla^\delta u_i^h \cdot \nabla\theta^h - \nabla^\delta u_i \cdot \nabla\theta - \nabla^\delta u_i \cdot \nabla\rho), \varphi). \end{aligned}$$

After eliminating the terms that vanish due to the definition of the elliptic projection, we obtain the following identity:

$$\begin{aligned} &(\partial_t\psi, \varphi) + (K\nabla\psi, \nabla\varphi) \\ &\quad = -(\partial_t\rho, \varphi) + \sum_{i=1}^N (T_i(\nabla^\delta u_i^h \cdot \nabla\theta^h - \nabla^\delta u_i \cdot (\nabla\theta + \nabla\rho)), \varphi). \end{aligned} \tag{59}$$

We can deal with the second term on the right hand side of (59) as follows:

$$\begin{aligned} &\nabla^\delta u_i^h \cdot \nabla\theta^h - \nabla^\delta u_i \cdot \nabla\theta - \nabla^\delta u_i \cdot \nabla\rho \\ &\quad = (\nabla^\delta u_i^h - \nabla^\delta u_i) \cdot \nabla\theta^h + \nabla^\delta u_i \cdot (\nabla\theta^h - \nabla\theta - \nabla\rho) \\ &\quad = (\nabla^\delta u_i^h - \nabla^\delta u_i)(\nabla\psi + \nabla\tilde{\theta}^h) + \nabla^\delta u_i \cdot \nabla\psi \end{aligned}$$

Now using $\varphi := \psi$ as a test function and relying on the bound

$$\|\nabla\tilde{\theta}^h\|_\infty < C(\theta)$$

(available cf. Lemma 4.6), we obtain:

$$\frac{1}{2}\partial_t\|\psi\|^2 + m\|\nabla\psi\|^2 \leq \frac{1}{2}\|\partial_t\rho\|^2 + \frac{1}{2}\|\psi\|^2 + \sum_{i=1}^{N}(C\|u_i^h - u_i\|^2 + \varepsilon\|\nabla\psi\|^2 + \varepsilon\|u_i\|_\infty(\|\nabla\rho\|^2 + \|\nabla\psi\|^2) + \|\psi\|^2).$$

Gronwall's inequality gives

$$\|\psi(t)\|^2 \leq \|\psi(0)\|^2 + C\int_0^t (\|\partial_t\rho\|^2 + \|\nabla\rho\|^2 + \sum_{i=1}^{N}\|u_i^h - u_i\|^2).$$

The estimate

$$\|\psi(0)\| \leq \|\theta^{h,0} - \theta^0\| + \|\tilde{\theta}^h(0) - \theta^0\| \leq \|\theta^{h,0} - \theta^0\| + Ch^2\|\theta^0\|_2,$$

together with the estimate $\|u_i^h - u_i\| \leq C(u)h^2$ give the statement of the Theorem. □

5. Fully discrete error analysis

Let $\tau > 0$ to be a small enough time step and use $t_n := \tau n$ while denoting $\theta^n := \theta(t_n)$ and $u_i^n := u_i(t_n)$. The discrete in space approximations of θ^n and u_i^n are denoted as $\theta^{h,n}$ and $u_i^{h,n}$, respectively.

Definition 5. *The triplet $(\theta^{h,n}, u_i^{h,n}, v_i^{h,n})$ is a discrete solution to (5)-(13) if the following identities hold for all $n \in \{1, \dots, N\}$ and $\varphi \in S_h$:*

$$\frac{1}{\tau}(\theta^{h,n+1} - \theta^{h,n}, \varphi) + (K\nabla\theta^{h,n+1}, \nabla\varphi) - \sum_{i=1}^{N}(T_i\nabla^\delta u_i^{h,n} \cdot \nabla\theta^{h,n+1}, \varphi) = 0, \tag{60}$$

$$\frac{1}{\tau}(u_i^{h,n+1} - u_i^{h,n}, \varphi) + (D_i\nabla u_i^{h,n+1}, \nabla\varphi) - (F_i\nabla^\delta\theta^{h,n} \cdot \nabla u_i^{h,n+1}, \varphi) + (A_i u_i^{h,n+1} - B_i v_i^{h,n+1}, \varphi) = (R_i(u^{h,n}), \varphi), \tag{61}$$

$$\frac{1}{\tau}(v_i^{h,n+1} - v_i^{h,n}, \varphi) = (A_i u_i^{h,n+1} - B_i v_i^{h,n+1}, \varphi), \tag{62}$$

$$\theta^{h,0} = \theta^{0,h}, \tag{63}$$

$$u_i^{h,0} = u_i^{0,h}, \tag{64}$$

$$v_i^{h,0} = v_i^{0,h}. \tag{65}$$

Here, $\theta^{0,h}$, $u_i^{0,h}$, and $v_i^{0,h}$ are the approximations of θ^0, u_i^0, and v_i^0 respectively in the finite dimensional space S_h.

Remark 5.1. *To treat (60) and (61), we use a semi-implicit discretization very much in the spirit of Ref. [33]. Note however that other options for time discretization are possible.*

Theorem 5.2. *Let (θ, u_i, v_i) solve (16)-(19) and (θ^h, u_i^h, v_i^h) solve (60)-(65), and assumptions (A_1)-(A_2) hold. Then the following inequality holds:*

$$\begin{aligned} &\|\theta^{h,n} - \theta^n\| + \sum_{i=1}^{N} \|u_i^{h,n} - u_i^n\| + \sum_{i=1}^{N} \|v_i^{h,n} - v_i^n\| \\ &\quad \leq C_1 \|\theta^{h,0} - \theta^0\| + C_2 \sum_{i=1}^{N} \|u_i^{h,0} - u_i^0\| + C_3 \sum_{i=1}^{N} \|v_i^{h,0} - v_i^0\| \\ &\quad + C_4(h^2 + \tau). \end{aligned} \tag{66}$$

The constants $C_1, \ldots, C_4$ entering (66) depend on controllable norms of θ, u_i, but are independent of h and τ.

Proof. Similar with the methodology of the proof of the semidiscrete *a priori* error estimates, we split the error terms into two parts:

$$\theta^{h,n} - \theta^n = \rho^{\theta,n} + \psi^{\theta,n} := (\theta^{h,n} - R_h\theta^n) + (R_h\theta^n - \theta^n), \tag{67}$$

$$u_i^{h,n} - u_i^n = \rho^{u_i,n} + \psi^{u_i,n} := (u_i^{h,n} - R_h u_i^n) + (R_h u_i^n - u_i^n), \tag{68}$$

where $R_h\theta$ and $R_h u_i$ are the Ritz projections defined by:

$$(K\nabla(R_h\theta - \theta), \nabla\varphi) = 0, \qquad \forall \varphi \in S_h, \tag{69}$$

$$(D_i\nabla(R_h u_i - u_i), \nabla\varphi) = 0, \qquad \forall \varphi \in S_h, i \in \{1, \ldots, N\}. \tag{70}$$

Here, $\psi^{\theta,n}$ and $\psi^{u_i,n}$ satisfy the following bounds:

$$\|\psi^{\theta,n}\| \leq Ch^2 \|\theta^n\|_2, \tag{71}$$

$$\|\psi^{u_i,n}\| \leq Ch^2 \|u_i^n\|_2, \tag{72}$$

so it remains to bound from above $\rho^{\theta,n}$ and $\rho^{u_i,n}$. We can write for $\rho^{\theta,n}$ the following identities:

$$\begin{aligned} &\frac{1}{\tau}(\rho^{\theta,n+1} - \rho^{\theta,n}, \varphi) + (K\nabla\rho^{\theta,n+1}, \nabla\varphi) = \frac{1}{\tau}(\theta^{h,n+1} - \theta^{h,n}, \varphi) + (K\nabla\theta^{h,n+1}, \nabla\varphi) \\ &\quad - \sum_{i=1}^{N} (T_i \nabla^\delta u_i^{h,n} \cdot \nabla\theta^{h,n+1}, \varphi) + \sum_{i=1}^{N} (T_i \nabla^\delta u_i^{h,n} \cdot \nabla\theta^{h,n+1}, \varphi) \\ &\quad - \frac{1}{\tau}(R_h\theta^{n+1} - R_h\theta^n, \varphi) - (K\nabla R_h\theta^{n+1}, \nabla\varphi) \\ &= \sum_{i=1}^{N} (T_i \nabla^\delta u_i^{h,n} \cdot \nabla\theta^{h,n+1}, \varphi) - \frac{1}{\tau}(R_h\theta^{n+1} - R_h\theta^n, \varphi) - (K\nabla\theta^{n+1}, \nabla\varphi) \\ &= \sum_{i=1}^{N} (T_i \nabla^\delta u_i^{h,n} \cdot \nabla\theta^{h,n+1}, \varphi) - \frac{1}{\tau}(R_h\theta^{n+1} - R_h\theta^n, \varphi) \\ &\quad + (\partial_t\theta^{n+1}, \varphi) - \sum_{i=1}^{N} (T_i \nabla^\delta u_i^{n+1} \cdot \nabla\theta^{n+1}, \varphi). \end{aligned}$$

After re-arranging the terms in the former expression, we obtain:

$$\begin{aligned}
&\frac{1}{\tau}(\rho^{\theta,n+1}-\rho^{\theta,n},\varphi)+(K\nabla\rho^{\theta,n+1},\nabla\varphi)\\
&\quad=\underbrace{\sum_{i=1}^{N}(T_i(\nabla^\delta u_i^{h,n}\cdot\nabla\theta^{h,n+1}-\nabla^\delta u_i^{n+1}\cdot\nabla\theta^{n+1}),\varphi)}_{A}\\
&\quad+\underbrace{(\partial_t\theta^{n+1}-\frac{1}{\tau}(\theta^{n+1}-\theta^n),\varphi)}_{B}-\underbrace{\frac{1}{\tau}(\psi^{\theta,n+1}-\psi^{\theta,n},\varphi)}_{C}.
\end{aligned}$$

Let us deal first with estimating the term C, then B, and finally, the term A.

To estimate the term C, we use our semidiscrete estimate for $\|\partial_t\psi\|$ stated in Lemma 4.5, we get:

$$\|\frac{1}{\tau}(\psi^{\theta,n+1}-\psi^{\theta,n})\|=\|\frac{1}{\tau}\int_{t^n}^{t^{n+1}}\partial_t\psi^\theta\|\le C_C(\theta,u)h^2.$$

The term B can be estimated as follows:

$$B=(\frac{1}{\tau}\int_{t^n}^{t^{n+1}}(s-t^n)\partial_{tt}\theta(s)ds,\varphi)\le\frac{\tau}{2}(\sup_{[t^n,t^{n+1}]}|\partial_{tt}\theta|)\|\varphi\|=C_B(\theta)\tau\|\varphi\|.$$

Finally, to tackle the term A, we proceed as follows:

$$\begin{aligned}
A&=(\nabla^\delta u_i^{h,n}\cdot\nabla\theta^{h,n+1}-\nabla^\delta u_i^{n+1}\cdot\nabla\theta^{n+1},\varphi)\\
&=(\nabla^\delta u_i^{h,n}\cdot(\nabla\theta^{h,n+1}-\nabla\theta^{n+1})+\nabla\theta^{n+1}\cdot(\nabla^\delta u_i^{h,n}-\nabla^\delta u_i^{n+1}),\varphi)\\
&\le\varepsilon\|u_i^{h,n}\|_\infty(\|\nabla\rho^{n+1}\|^2+\|\nabla\psi^{n+1}\|^2)+C_\varepsilon\|\varphi\|^2\\
&\quad+\underbrace{(\nabla\theta^{n+1}\cdot(\nabla^\delta u_i^{h,n}-\nabla^\delta u_i^{n+1}),\varphi)}_{D}.
\end{aligned}$$

At its turn, the term D can be expressed as:

$$\begin{aligned}
D&=(\nabla\theta^{n+1}\cdot(\nabla^\delta u_i^{h,n}-\nabla^\delta u_i^n),\varphi)+(\nabla\theta^{n+1}\cdot(\nabla^\delta u_i^n-\nabla^\delta u_i^{n+1}),\varphi)\\
&\le\|\nabla\theta^{n+1}\|_\infty(\varepsilon\|\nabla^\delta(u_i^{h,n}-u_i^n)\|^2+C_\varepsilon\|\varphi\|^2)+\underbrace{(\nabla\theta^{n+1}\cdot\int_{t^n}^{t^{n+1}}\partial_t\nabla^\delta u_i,\varphi)}_{E}.
\end{aligned}$$

Finally, the term E can be estimated as:

$$E\le\|\nabla\theta^{n+1}\|_\infty\|\partial_t\nabla^\delta u_i\|_\infty\tau\|\varphi\|.$$

Adding together all the terms, and then substituting $\varphi:=\rho^{\theta,n+1}$ we finally obtain:

$$\begin{aligned}
&\frac{1}{\tau}\|\rho^{\theta,n+1}\|^2+m\|\nabla\rho^{\theta,n+1}\|^2\le\frac{1}{\tau}\|\rho^{\theta,n}\|^2+(C_B(\theta)\tau)^2\\
&\quad+(C_C(\theta)h^2)^2+\varepsilon\|u_i^{h,n}\|_\infty(\|\nabla\rho^{\theta,n+1}\|^2+\|\nabla\psi^{n+1}\|^2)\\
&\quad+C_D\varepsilon\|\nabla^\delta(u_i^{h,n}-u_i^n)\|^2+(C_E(u,\theta)\tau)^2+C\|\rho^{\theta,n+1}\|^2\\
&\quad:=C\|\rho^{\theta,n+1}\|^2+R_n, \qquad (73)
\end{aligned}$$

where the reminder R_n is defined by:

$$R_n := \frac{1}{\tau}\|\rho^{\theta,n}\|^2 + (C_B(\theta)\tau)^2 + (C_C(\theta)h^2)^2 + \varepsilon\|u_i^{h,n}\|_\infty(\|\nabla\rho^{\theta,n+1}\|^2 + \|\nabla\psi^{n+1}\|^2)$$
$$+ C_D\varepsilon\|\nabla^\delta(u_i^{h,n} - u_i^n)\|^2 + (C_E(u,\theta)\tau)^2$$

For R_n it holds:

$$R_n \le C(\theta,u)(h^2+\tau)^2.$$

Note that we can derive a similar estimate for $\rho^{u_i,n+1}$, which we then add to (73).

To conclude, we denote

$$e^n := \|\rho^{\theta,n}\|^2 + \sum_{i=1}^N \|\rho^{u_i,n}\|^2,$$

to obtain the short structure

$$\frac{1}{\tau}e^{n+1} \le \frac{1}{\tau}e^n + C(e^{n+1} + R_n).$$

From here it follows that:

$$(1 - C\tau)e^{n+1} \le e^n + C\tau R_n.$$

For sufficiently small τ, we can instead write the expression

$$e^{n+1} \le (1 + C\tau)e^n + C\tau R_n.$$

Iterating the later inequality, we obtain

$$e^{n+1} \le (1 + C\tau)^{n+1}e^0 + C\tau\sum_{j=1}^n R_j.$$

Finally, this argument yields

$$e^{n+1} \le C\|\theta^{h,0} - \theta^0\| + C\|u_i^{h,0} - u_i^0\| + C(\theta,u)(h^2+\tau),$$

which proves the Theorem 5.2. □

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