Discontinuous Galerkin Methods for fast reactive mass transfer through semi-permeable membranes

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Abstract

A discontinuous Galerkin (dG) method for the numerical solution of initial/boundary value multi-compartment partial differential equation (PDE) models, interconnected with interface conditions, is analysed. The study of interface problems is motivated by models of mass transfer of solutes through semi-permeable membranes. The case of fast reactions is also included. More specifically, a model problem consisting of a system of semilinear parabolic advection-diffusion-reaction partial differential equations in each compartment with only local Lipschitz conditions on the nonlinear reaction terms, equipped with respective initial and boundary conditions, is considered. General nonlinear interface conditions modelling selective permeability, congestion and partial reflection are applied to the compartment interfaces. The interior penalty dG method for this problem, presented recently, is analysed both in the space-discrete and in fully discrete settings for the case of, possibly, fast reactions. The a priori analysis shows that the method yields optimal a priori bounds, provided the exact solution is sufficiently smooth. Numerical experiments indicate agreement with the theoretical bounds.

1. Introduction

Models of mass transfer of substances (solutes) through semi-per-meable membranes appear in various contexts, such as biomedical and chemical engineering applications [20]. Examples include the modelling of electrokinetic flows (see, e.g., [6] and the references therein), cellular signal transduction (see, e.g., [12] and the references therein), and the modelling of solute dynamics across arterial walls (see, e.g., [30] and the references therein).

This work is concerned with the development and analysis of fully discrete discontinuous Galerkin methods for a class of continuum models for mass transfer based on initial/boundary value multi-compartment partial differential equation (PDE) problems, closed by nonlinear Kedem-Katchalsky (KK) interface conditions [23, 22]. Finite element methods for mass transfer models have been developed for the solution of solute dynamics across arterial walls; see [30, 29, 28] and the references therein, while existence results for the purely diffusing interface problem coupled with KK-type interface conditions are given in [10]. Further, numerical approaches to the treatment of interface conditions for PDE problems, resulting to globally continuous solutions can be found, e.g., in [5, 2, 13, 27, 25]. The advantages of dG methods for interfacing different numerical methods (numerical interfaces) have been identified [26, 15], as well as their use on transmission-type/high-contrast problems, yielding continuous solutions across the transmission interface, has been investigated [17, 8, 18, 9].

This work builds upon the recent numerical treatment of this class of problems presented in [11]. There, a dG method for the same problem is presented along with an a priori error analysis for the space-discrete case, utilising a continuation argument, in conjunction with a non-standard elliptic projection inspired by a classical construction of Douglas and Dupont [16] for the treatment of nonlinear boundary conditions. The continuation argument used in [11] was able to deliver optimal a priori bounds with respect to the local mesh-size, without the need of global mesh quasi-uniformity assumptions (cf. [24]), at the expense of covering a more restrictive range of nonlinear growth in the reaction terms. Here, we extend the a priori error analysis for the same method under the weaker assumption of only local Lipschitz growth of the reaction terms. As, perhaps, expected this is achieved at the expense of stricter mesh assumptions: roughly speaking, these are assumptions of the form $h_{\min}^{-d/2}h_{\max}^{s-1}$, where $h_{\min}$ and $h_{\max}$ are the smallest and largest element diameters across a given mesh, d is the spatial dimension and s is the optimal rate of approximation of finite element-type functions in the L^2 norm. The fixed point argument used has been applied to other types of finite element methods for time-dependent semilinear problems, *cf.* for instance [1, 19].

The remaining of this work is organized as follows. In Section 2, the PDE model is detailed, while in Section 3 we review the dG method proposed for the advection-diffusion part of the spatial operator incorporating the nonlinear interface conditions. Two a priori error bounds are presented in Section 4 , one for the spatially discrete case and one for the fully discrete case. Finally, Section 6 contains some numerical experiments.

2. Model problem

We consider systems of parabolic semilinear PDEs on two disjoint subdomains Ω^1 and Ω^2 of $\mathbb{R}^d$, $d \in \{2,3\}$, coupled by nonlinear Neumann conditions at the *interface* $\Gamma_{\mathfrak{I}}$ between the subdomains.

For $n \in \mathbb{N}$, we define the *broken* space $\mathbb{H}^s := [H^s(\Omega^1 \cup \Omega^2)]^n$, $s \in \mathbb{R}$, and introduce the model problem:

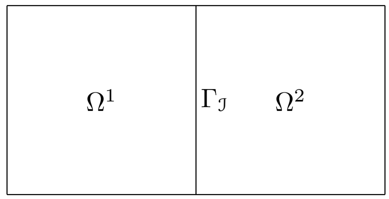

Figure 1: The domain of solution is given by the two subdomains Ω^1, Ω^2 joining at the internal boundary $\Gamma_{\mathcal{J}}$.

Find $\mathbf{u} \in L^2(0,T;\mathbb{H}^s)$, $s > 3/2$, with $\mathbf{u}_t \in L^2(0,T;\mathbb{H}^{-1})$ such that

$$
\begin{aligned}
&\mathbf{u}_t - \nabla \cdot (A\nabla \mathbf{u} - U\mathbf{B}) + \mathbf{F}(\mathbf{u}) = \mathbf{0} && \text{in } (0,T] \times (\Omega^1 \cup \Omega^2), && (1)\\
&\mathbf{u}(0,x) = \mathbf{u}_0(x) && \text{on } \{0\} \times \Omega, && (2)\\
&\mathbf{u} = \mathbf{g}_{\mathrm{D}} && \text{on } \Gamma_{\mathrm{D}}, && (3)\\
&\big(A\nabla \mathbf{u} - \mathcal{X}^- U\mathbf{B}\big)\mathbf{n}|_{\Omega} = \mathbf{g}_{\mathrm{N}} && \text{on } \Gamma_{\mathrm{N}}, && (4)\\
&(A\nabla \mathbf{u} - U\mathbf{B})\,\mathbf{n}|_{\Omega^1} = \mathbf{g}_{\mathcal{J}}(\mathbf{u}^1, \mathbf{u}^2) && \text{on } \Gamma_{\mathcal{J}}, && (5)\\
&(A\nabla \mathbf{u} - U\mathbf{B})\,\mathbf{n}|_{\Omega^2} = -\mathbf{g}_{\mathcal{J}}(\mathbf{u}^1, \mathbf{u}^2) && \text{on } \Gamma_{\mathcal{J}}, && (6)
\end{aligned}
$$

where $\mathbf{u}^j := \mathbf{u}|_{\bar{\Omega}_j \cap \Gamma_{\mathcal{J}}}$, $j = 1,2$. Further, $\Omega = \Omega^1 \cup \Omega^2 \cup \Gamma_{\mathcal{J}}$ and $\mathbf{n}$ always denotes the unit normal vector pointing outward of the given domain boundary. For $i = 1,2$, we assume that Ω^i has Lipschitz boundary and that $\partial\Omega^i \cap \partial\Omega$ has positive $(d-1)$-dimensional (Hausdorff) measure. See Figure 1 for an exemplification of the solution domain.

We employ the following notational convention: vectors are indicated with lower case bold symbols, $n \times n$ diagonal matrices with upper case (non-bold) symbols, and $n \times d$ tensors with upper case bold symbols. The gradient $\nabla \mathbf{v}$ of a vector function $\mathbf{v} : \Omega^1 \cup \Omega^2 \to \mathbb{R}^n$ in $\mathbb{H}^1$ is a mapping $\Omega^1 \cup \Omega^2 \to \mathbb{R}^{n\times d}$ gained from component-wise application of the gradient operation: $\nabla \mathbf{v} := (\nabla v_1, \dots, \nabla v_n)^{\mathsf{T}}$. Similarly the divergence $\nabla \cdot \mathbf{Q}$ of the tensor-valued function $\mathbf{Q} : \Omega^1 \cup \Omega^2 \to \mathbb{R}^{n\times d}$ is $\nabla \cdot \mathbf{Q} := (\nabla \cdot Q_1, \dots, \nabla \cdot Q_n)^{\mathsf{T}}$ where the Q_i are rows of $\mathbf{Q}$. Finally, $U = \mathrm{diag}(\mathbf{u})$.

The data of the problem are defined as follows. The field $\mathbf{B}$ is an $n \times d$ tensor with rows $B_i \in C^1(0,T;W^{1,\infty}(\Omega\backslash\Gamma_{\mathcal{J}})^d \cap W^{\infty}(\mathrm{div},\Omega))$, $i = 1,\dots,n$, and $A \in [C([0,T]\times\Omega^1\cup\Omega^2)]^{n\times n}$ diagonal, with $A = \mathrm{diag}(a_1, a_2, \dots, a_n)$, where $a_i : [0,T] \times \Omega^1 \cup \Omega^2 \to \mathbb{R}$, $i = 1,\dots,n$. We assume that there exists a constant $\alpha_{\min} > 0$ of uniform parabolicity such that $a_i(t,x) \geq \alpha_{\min}$ for all $i = 1,\dots,n$ and $(t,x) \in [0,T] \times \Omega$. For simplicity, we also require that the matrix $\mathrm{diag}(\nabla \cdot \mathbf{B})$ is positive semi-definite. Finally, $\mathbf{F} : \mathbb{R}^n \to \mathbb{R}^n$ is a vector field satisfying a Lipschitz condition on every compact set of $\mathbb{R}^n$. We stress, that *no* global Lipschitz continuity is assumed.

The boundary $\partial\Omega$ is split into $\partial\Omega = \Gamma_{\mathrm{D}} \cup \Gamma_{\mathrm{N}}$, with Γ_{D} being of positive $(d-1)$-dimensional (Hausdorff) measure. Further, we subdivide $\partial\Omega = \partial\Omega_i^- \cup \partial\Omega_i^+$, where $\partial\Omega_i^- := \{\mathbf{x} \in \partial\Omega : (B_i\mathbf{n})(\mathbf{x}) < 0\}$ and $\partial\Omega_i^+ = \partial\Omega\backslash\partial\Omega_i^-$ are the *inflow* and *outflow* parts of the boundary $\partial\Omega$ for the i-th equation. We denote by $\chi_i^- : \partial\Omega_i^- \to \mathbb{R}$ the characteristic function of $\partial\Omega_i^-$; further $\mathcal{X}^- := \mathrm{diag}(\chi_1^-, \dots, \chi_n^-)$, and $\mathcal{X}^+ := I -$

$\mathcal{X}^-$. The Dirichlet and Neumann data are $\mathbf{g}_\mathrm{D} \in H^{1/2}(\Gamma_\mathrm{D})^n$ and $\mathbf{g}_\mathrm{N} \in L^2(\Gamma_\mathrm{N})^n$, respectively.

The problems on Ω^1 and Ω^2 are coupled by the interface conditions (5) and (6). These state that the flux across the interface is continuous and is a given function of the solution traces at the interface. We assume that the flux function $\mathbf{g}_\mathcal{J}$ takes the form

$$\mathbf{g}_\mathcal{J}(\mathbf{u}^1, \mathbf{u}^2) = \tilde{\mathbf{p}}(\mathbf{u}^1, \mathbf{u}^2) - \mathrm{R}(\Upsilon^1 U^1 + \Upsilon^2 U^2)(\mathbf{B}\mathbf{n})|_{\Omega^1}, \quad \text{on } \Gamma_\mathcal{J}. \tag{7}$$

Here, $\tilde{\mathbf{p}} : \mathbb{R}^{2n} \to \mathbb{R}^n$ is a general function of the traces of $\mathbf{u}$ from both sides of the interface and thus cover a number of known membranes models [23, 22, 30, 6, 11]. For instance, a typical diffusion phenomenon would yield a term proportional to the solution jump at the interface, with the constant of proportionality given by the membrane *permeability*, cf. [11]. The second term in (7) describes the net advection through the interface in terms of the friction coefficients and weights $\Upsilon^j = \mathrm{diag}(\upsilon_1^j, \dots, \upsilon_n^j)$, $j = 1, 2$ and $\mathrm{R} = \mathrm{diag}(r_1, \dots, r_n)$ with $r_i, \upsilon_i^{1,2} : \Gamma_\mathcal{J} \to [0, 1]$ and $i = 1, \dots, n$.

In view of the analysis below, we make the following (physically reasonable) assumptions. We assume that $\tilde{\mathbf{p}} \in C^{1,1}(\mathbb{R}^{2n})$ and that its Jacobian $\tilde{\mathbf{p}}'$ is uniformly bounded. Further, for every $i = 1, \dots, n$, the weights $\upsilon_i^{1,2}$ satisfy, for any $\mathbf{x} \in \Gamma_\mathcal{J}$,

$$\upsilon_i^1(\mathbf{x}) + \upsilon_i^2(\mathbf{x}) = 1, \qquad \begin{cases} \upsilon_i^1(\mathbf{x}) \geq \upsilon_i^2(\mathbf{x}) & \text{if } (B_i \mathbf{n}|_{\partial\Omega^1})(\mathbf{x}) \geq 0, \\ \upsilon_i^1(\mathbf{x}) < \upsilon_i^2(\mathbf{x}) & \text{otherwise.} \end{cases} \tag{8}$$

Throughout this work, we shall assume that the above system has a unique solution that remains bounded up to, and including, the final time T.

3. The discontinuous Galerkin method

3.1. Finite element spaces

Let $\mathcal{T}$ be a shape-regular and locally quasi-uniform subdivision of Ω into disjoint open elements $\kappa \in \mathcal{T}$, such that $\Gamma_\mathcal{J} \subset \cup_{\kappa\in\mathcal{T}} \partial\kappa =: \Gamma$, the *skeleton*. Further we decompose Γ into three disjoint subsets $\Gamma = \partial\Omega \cup \Gamma_\mathrm{int} \cup \Gamma_\mathcal{J}$, where $\Gamma_\mathrm{int} := \Gamma \backslash (\partial\Omega \cup \Gamma_\mathcal{J})$. We assume that the subdivision $\mathcal{T}$ is constructed via mappings F_κ, where $F_\kappa : \hat{\kappa} \to \kappa$ are smooth maps with non-singular Jacobian, and $\hat{\kappa}$ is the reference d-dimensional simplex or the reference d-dimensional (hyper)cube. It is assumed that the union of the closures of the elements $\kappa \in \mathcal{T}$ forms a covering of the closure of Ω; i.e., $\bar{\Omega} = \cup_{\kappa\in\mathcal{T}} \bar{\kappa}$.

For $m \in \mathbb{N}$ we denote by $\mathbb{P}_m(\hat{\kappa})$ the set of polynomials of total degree at most m if $\hat{\kappa}$ is the reference simplex, and the set of all tensor-product polynomials on $\hat{\kappa}$ of degree k in each variable, if $\hat{\kappa}$ is the reference hypercube. Let $m_\kappa \in \mathbb{N}$ be given for each $\kappa \in \mathcal{T}$. We consider the hp-discontinuous finite element space

$$\mathrm{V}_h := \{v \in L^2(\Omega) : v|_\kappa \circ F_\kappa \in \mathbb{P}_{m_\kappa}(\hat{\kappa}),\ \kappa \in \mathcal{T}\}, \tag{9}$$

and set $\mathbb{V}_h := [\mathrm{V}_h]^n$.

Next, we introduce relevant trace operators. Let κ^+, κ^- be two elements sharing an edge $e := \partial\kappa^+ \cap \partial\kappa^- \subset \Gamma_\mathrm{int} \cup \Gamma_\mathcal{J}$. Denote the outward normal unit vectors on e of $\partial\kappa^+$ and $\partial\kappa^-$ by $\mathbf{n}^+$ and $\mathbf{n}^-$, respectively. For functions $\mathbf{q} : \Omega \to \mathbb{R}^n$ and

$\mathbf{Q} : \Omega \to \mathbb{R}^{n\times d}$ that may be discontinuous across Γ, we define the following quantities: for $\mathbf{q}^+ := \mathbf{q}|_{\kappa^+}$, $\mathbf{q}^- := \mathbf{q}|_{\kappa^-}$ and $\mathbf{Q}^+ := \mathbf{Q}|_{\kappa^+}$, $\mathbf{Q}^- := \mathbf{Q}|_{\kappa^-}$ on the restriction to e, we set

$$\{\mathbf{q}\} := \frac{1}{2}(\mathbf{q}^+ + \mathbf{q}^-), \qquad \{\mathbf{Q}\} := \frac{1}{2}(\mathbf{Q}^+ + \mathbf{Q}^-),$$

and

$$[\![\mathbf{q}]\!] := \mathbf{q}^+ \otimes \mathbf{n}^+ + \mathbf{q}^- \otimes \mathbf{n}^-, \qquad [\mathbf{Q}] := \mathbf{Q}^+\mathbf{n}^+ + \mathbf{Q}^-\mathbf{n}^-,$$

where $\otimes$ denotes the standard tensor product operator, with $\mathbf{q} \otimes \mathbf{w} = \mathbf{q}\mathbf{w}^\mathsf{T}$. If $e \in \partial\kappa \cap \partial\Omega$, these definitions are modified as follows: $\{\mathbf{q}\} := \mathbf{q}^+$, $\{\mathbf{Q}\} := \mathbf{Q}^+$ and $[\![\mathbf{q}]\!] := q^+ \otimes \mathbf{n}$, $[\mathbf{Q}] := \mathbf{Q}^+\mathbf{n}$.

Further, we introduce the mesh quantities $\mathtt{h} : \Omega \to \mathbb{R}$, $\mathtt{m} : \Omega \to \mathbb{R}$ with $\mathtt{h}(x) = \operatorname{diam}\kappa$, $\mathtt{m}(x) = m_\kappa$, if $x \in \kappa$, and the averaged values $\mathtt{h}(x) = \{\mathtt{h}\}$, $\mathtt{m}(x) = \{\mathtt{m}\}$, if $x \in \Gamma$. Finally, we define $h_{\max} := \max_{x\in\Omega} \mathtt{h}$ and $h_{\min} := \min_{x\in\Omega} \mathtt{h}$.

We shall assume the existence of a constant $C_A \geq 1$ independent of $\mathcal{T}$ such that, on any face that is *not* contained in $\Gamma_\mathcal{I}$, given the two elements κ, κ' sharing that face, the diffusion matrix A satisfies

$$C_A^{-1} \leq \big\|A\|_{\infty,\kappa}\|A^{-1}\big\|_{\infty,\kappa'} \leq C_A. \tag{10}$$

We refer to [18] on possible ways to remove this assumption; we refrain from doing so here for simplicity of the presentation. The next result is a modification of the classical trace estimate for functions in $H^1(\Omega^1 \cup \Omega^2) + \mathrm{V}_h$; see [7] for similar results.

Lemma 1 ([11])**.** *Assume that the mesh $\mathcal{T}$ is both shape-regular and locally quasi-uniform. Then for $v \in H^1(\Omega^1 \cup \Omega^2) + \mathrm{V}_h$, the following trace estimate holds:*

$$\sum_{j=1}^{2} \|v|_{\Omega^j}\|^2_{\Gamma_\mathcal{I}} \leq c_1\epsilon\Big(\sum_{\kappa\in\mathcal{T}} \|\nabla v\|^2_\kappa + \|\mathtt{h}^{-1/2}[v]\|^2_{\Gamma_{\text{int}}}\Big) + c_2\epsilon^{-1}\|v\|^2, \tag{11}$$

for any $\epsilon > h_{\max}$ and for some constants $c_1 > 0$ and $c_2 > 0$, depending only on the shape-regularity of the mesh and on the domain Ω.

3.2. Space discretization

The following dG-in-space method for the system (1), (2), (3), (4), (5), and (6) has been introduced in [11], albeit for a slightly less general flux function. The discretization of the space variables was based on a dG method of interior penalty type for the diffusion part and of upwind type for the advection; moreover, special care had to be given to the incorporation of the interface conditions. The semi-discrete in space method reads:

For $t = 0$, let $\mathbf{u}_h(0) = \Pi\mathbf{u}_0$, with $\Pi : [L^2(\Omega)]^n \to \mathbb{V}_h$ denoting the orthogonal L^2-projection onto $\mathbb{V}_h$. For $t \in (0, T]$, find $\mathbf{u}_h \equiv \mathbf{u}_h(t) \in \mathbb{V}_h$ such that

$$\langle(\mathbf{u}_h)_t, \mathbf{v}_h\rangle + B(\mathbf{u}_h, \mathbf{v}_h) + N(\mathbf{u}_h, \mathbf{v}_h) + \langle\mathbf{F}(\mathbf{u}_h), \mathbf{v}_h\rangle = l(\mathbf{v}_h), \quad \text{for all} \quad \mathbf{v}_h \in \mathbb{V}_h, \tag{12}$$

where

$$
\begin{aligned}
B(\mathbf{u}_h,\mathbf{v}_h) &:= \sum_{\kappa\in\mathcal{T}}\int_\kappa (A\nabla\mathbf{u}_h - U_h\mathbf{B}) : \nabla\mathbf{v}_h + \int_{\Gamma_\mathcal{J}} \Big(\{U_h\mathbf{B}\} + \mathcal{B}_\mathcal{J}[\![\mathbf{u}_h]\!]\Big) : [\![\mathbf{v}_h]\!] \\
&- \int_{\Gamma_{\text{int}}} \Big(\{A\nabla\mathbf{u}_h - U_h\mathbf{B}\} : [\![\mathbf{v}_h]\!] + \{A\nabla\mathbf{v}_h\} : [\![\mathbf{u}_h]\!] - (\Sigma+\mathcal{B})[\![\mathbf{w}_h]\!] : [\![\mathbf{v}_h]\!]\Big) \\
&- \int_{\Gamma_\text{D}} \Big((A\nabla\mathbf{w}_h - \mathcal{X}^+U_h\mathbf{B}) : (\mathbf{v}_h\otimes\mathbf{n}) + (A\nabla\mathbf{v}_h) : (\mathbf{w}_h\otimes\mathbf{n}) - \Sigma\mathbf{w}_h\cdot\mathbf{v}_h\Big) \\
&+ \int_{\Gamma_\text{N}} (\mathcal{X}^+U_h\mathbf{B}) : (\mathbf{v}_h\otimes\mathbf{n}),
\end{aligned}
\tag{13}
$$

and

$$
N(\mathbf{u}_h,\mathbf{v}_h) := \int_{\Gamma_\mathcal{J}} \big(\tilde{\mathbf{p}}(\mathbf{u}_h^1,\mathbf{u}_h^2)\otimes\mathbf{n}|_{\Omega^2} - (\text{I}-\text{R})\left(\{U_h\mathbf{B}\} + \mathcal{B}_\mathcal{J}[\![\mathbf{u}_h]\!]\right)\big) : [\![\mathbf{v}_h]\!], \tag{14}
$$

and

$$
l(\mathbf{v}_h) := -\int_{\Gamma_\text{D}}\Big((\mathbf{g}_\text{D}\otimes\mathbf{n}) : (A\nabla\mathbf{v}_h) + (\mathcal{X}^-G_\text{D}\mathbf{B}) : (\mathbf{v}_h\otimes\mathbf{n}) - \Sigma\mathbf{g}_\text{D}\cdot\mathbf{v}_h\Big) + \int_{\Gamma_\text{N}} \mathbf{g}_\text{N}\cdot\mathbf{v}_h, \tag{15}
$$

with $G_\text{D} = \text{diag}(\mathbf{g})$, $U_h := \text{diag}(\mathbf{u}_h)$, and $\Sigma := C_\sigma A\mathtt{m}^2\mathtt{h}^{-1}$ denoting the *discontinuity-penalization parameter* matrix with $C_\sigma > 1$ constant. Furthermore,

$$
\mathcal{B} := \frac{1}{2}\,\text{diag}(|B_1\cdot\mathbf{n}|,\ldots,|B_n\cdot\mathbf{n}|),
$$

and

$$
\mathcal{B}_\mathcal{J} := (\Upsilon^1 - \frac{1}{2}\text{I})\mathbf{Bn}|_{\Omega^1} = (\Upsilon^2 - \frac{1}{2}\text{I})\mathbf{Bn}|_{\Omega^2}
$$

is diagonal with non negative entries.

To ensure the coercivity of B, the advective interface term has been split as

$$
\text{R} = \text{I} - (\text{I}-\text{R}),
$$

resulting into contributions in both B and N. In this way, the advective interface contribution in B can be recast using the weighted mean $\{W_h\mathbf{B}\}^\upsilon := \Upsilon^1 W_h\mathbf{B}|_{\Omega^1} + \Upsilon^2 W_h\mathbf{B}|_{\Omega^2}$, so that

$$
\{W_h\mathbf{B}\}^\upsilon : [\![\mathbf{v}_h]\!] = (\{W_h\mathbf{B}\} + \mathcal{B}_\mathcal{J}[\![\mathbf{w}_h]\!]) : [\![\mathbf{v}_h]\!], \tag{16}
$$

thereby resembling the typical dG upwinding for linear advection problem.

Notice also that, if the flux function takes the particular form considered in [11], namely $\tilde{\mathbf{p}}(\mathbf{u}^1,\mathbf{u}^2)\otimes\mathbf{n}|_{\Omega^2} = \mathbf{P}(\mathbf{u}^1,\mathbf{u}^2)[\![\mathbf{u}]\!]$ for some *permeability* tensor $\mathbf{P}$, then the diffusion term appearing in N is simply given by $\int_{\Gamma_\mathcal{J}}\mathbf{P}(\mathbf{w})[\![\mathbf{w}]\!] : [\![\mathbf{v}_h]\!]$. This resembles the typical jump stabilisation term with the permeability coefficient replacing the discontinuity-penalization parameter.

3.3. Elliptic projection

A nonlinear elliptic projection inspired by a classical construction of Douglas and Dupont [16] for the treatment of nonlinear boundary conditions, was developed in [11]. Here we review some of these developments that are necessary in the error analysis below. For the proofs, we refer to [11].

Definition 1. *For each $t \in [0,T]$ we define the* elliptic projection $\mathbf{w}_h \in \mathbb{V}_h$ *to be the solution of the problem: find $\mathbf{w}_h \equiv \mathbf{w}_h(t) \in \mathbb{V}_h$, such that*

$$B(\mathbf{u}-\mathbf{w}_h,\mathbf{v}_h)+\lambda\langle\mathbf{u}-\mathbf{w}_h,\mathbf{v}_h\rangle+N(\mathbf{u},\mathbf{v}_h)-N(\mathbf{w}_h,\mathbf{v}_h)=0 \quad \forall\mathbf{v}_h\in\mathbb{V}_h, \tag{17}$$

for some fixed $\lambda > 0$.

The constant $\lambda > 0$ in the definition above is to be chosen large enough to ensure the uniqueness of the projection $\mathbf{w}_h$ (see [11] for details).

Next, denoting by $\mathbb{S}^s := \mathbb{H}^s + \mathbb{V}_h$, $s \in \mathbb{R}$, we define the dG-norm on $\mathbb{S}^1$

$$\begin{aligned} |||\mathbf{w}||| := \Bigg(\sum_{\kappa\in\mathcal{T}} \big(\|\sqrt{A}\nabla\mathbf{w}\|_\kappa^2 + \frac{1}{2}\|\sqrt{\operatorname{diag}(\nabla\cdot\mathbf{B})}\mathbf{w}\|_\kappa^2 \big) + \|\sqrt{\Sigma}[\![\mathbf{w}]\!]\|^2_{\Gamma_{\mathrm{D}}\cup\Gamma_{\mathrm{int}}} \\ + \|\sqrt{\mathcal{B}}[\![\mathbf{w}]\!]\|^2_{\Gamma\setminus\Gamma_{\mathcal{I}}} + \|\sqrt{\mathcal{B}_{\mathcal{I}}}[\![\mathbf{w}]\!]\|^2_{\Gamma_{\mathcal{I}}} \Bigg)^{1/2}, \end{aligned} \tag{18}$$

where $\|\mathbf{Q}\|_\kappa := \big(\int_\kappa \sum_{i=1}^n |Q_i(x)|^2 \,\mathrm{d}x\big)^{1/2}$, denotes the Frobenius norm whenever $\mathbf{Q}$ is a $n \times d$ tensor. We assume that (18) is a norm. This is satisfied when standard assumptions on the solution in conjunction with the boundary conditions hold on each subdomain, e.g., $\Gamma_{\mathrm{D}} \cap \partial\Omega^j$ has positive $(d-1)$-dimensional (Hausdorff) measure for $j = 1, 2$. If the interface manifold $\Gamma_{\mathcal{I}}$ is not characteristic to the advection field, such hypotheses can be further relaxed. We shall also make the simplifying assumption that $\mathbf{B}$ is such that:

$$B_i \cdot \nabla(v_h)_i \in \mathrm{V}_h, \quad \text{for } i = 1,\dots,n, \tag{19}$$

for any function $\mathbf{v}_h := ((v_h)_1,\dots,(v_h)_n)^{\mathsf{T}} \in \mathbb{V}_h$. We refer to [21, 4], on ways to circumvent this assumption for the case of scalar linear advection-diffusion problems.

The next two results show the coercivity and the continuity of the bilinear form $B(\cdot,\cdot)$. Their proofs follow straightforward variations of well-known arguments (see, e.g., [3, 21]) and are, therefore, omitted for brevity.

Lemma 2. *For $\mathbf{v}_h \in \mathbb{V}_h$, there exists a positive constant C_{coer}, independent of $\mathbf{v}_h$, such that*

$$B(\mathbf{v}_h,\mathbf{v}_h) \ge C_{\mathrm{coer}}|||\mathbf{v}_h|||^2.$$

Lemma 3. *Let $\Pi : [L^2(\Omega)]^n \to \mathbb{V}_h$ denote the L^2-orthogonal projection onto $\mathbb{V}_h$. For any $\mathbf{w} \in \mathbb{H}^s$, $s > 3/2$ and $\mathbf{v}_h \in \mathbb{V}_h$ we have*

$$|B(\boldsymbol{\eta},\mathbf{v}_h)| \le C_{\mathrm{cont}}|||\boldsymbol{\eta}|||_{\mathcal{B}}|||\mathbf{v}_h|||,$$

with $C_{\mathrm{cont}} > 0$ constant, independent of $\mathbf{w}$ and of $\mathbf{v}_h$, where $\boldsymbol{\eta} := \mathbf{w} - \Pi\mathbf{w}$ and

$$|||\boldsymbol{\eta}|||_{\mathcal{B}} := \big(|||\boldsymbol{\eta}|||^2 + \|\Sigma^{-1/2}\{A\nabla\boldsymbol{\eta}\}\|^2_{\Gamma_{\mathrm{D}}\cup\Gamma_{\mathrm{int}}} + \|\sqrt{\mathcal{B}}\{\boldsymbol{\eta}\}\|^2_{\Gamma} + \|\sqrt{\mathcal{B}_{\mathcal{I}}}\{\boldsymbol{\eta}\}\|^2_{\Gamma_{\mathcal{I}}}\big)^{1/2}. \tag{20}$$

The next result establishes the well-posedness of the problem (17) and relevant approximation properties.

Lemma 4. *Assume that* $\mathbf{u} \in \mathbb{H}^s$*,* $s > 3/2$ *for all* $t \in (0,T]$*. For* $\lambda > 0$ *sufficiently large and for* $h_{\max}$ *sufficiently small, the variational problem (17) has a unique solution* $\mathbf{w}_h \in \mathbb{V}_h$ *for each* $t \in (0,T]$*. Moreover, the following bound holds:*

$$C_{\mathrm{coer}}|||\boldsymbol{\rho}|||^2 + \lambda\|\boldsymbol{\rho}\|^2 \leq |||\boldsymbol{\eta}|||^2_{\mathcal{B},\lambda}, \tag{21}$$

and, if also $\mathbf{u}_t \in \mathbb{H}^s$*, then*

$$C_{\mathrm{coer}}|||\boldsymbol{\rho}_t|||^2 + \lambda\|\boldsymbol{\rho}_t\|^2 \leq |||\boldsymbol{\eta}_t|||^2_{\mathcal{B},\lambda} + |||\boldsymbol{\eta}|||^2_{\mathcal{B},\lambda}, \tag{22}$$

where $\boldsymbol{\rho} := \mathbf{u} - \mathbf{w}_h$*,* $\boldsymbol{\eta} := \mathbf{u} - \Pi\mathbf{u}$*, and*

$$|||\boldsymbol{\eta}|||_{\mathcal{B},\lambda} := \left(C_c|||\boldsymbol{\eta}|||^2_{\mathcal{B}} + 7\lambda\|\boldsymbol{\eta}\|^2\right)^{1/2},$$

with $C_c := (4C^2_{\mathrm{cont}} + 3C^2_{\mathrm{coer}})/C_{\mathrm{coer}}$*.*

Remark 1. *The assumption "*$h_{\max}$ *sufficiently small" is required to counteract the lack of monotonicity/coercivity of the interface non-linearity. It can be quantified exactly in view the statement of Lemma 1 (cf., Lemma 3.1 in [11]), requiring* $\epsilon > h_{\max}$ *and, in turn,* ϵ *is required to be sufficiently small in an explicit fashion in the proof of Lemmas 4.4 and 4.5 in [11].*

We conclude this section with an L^2-error bound of the elliptic projection (17). This is obtained by an Aubin-Nitsche duality-type argument, inspired by a construction of Douglas and Dupont [16] for nonlinear boundary conditions.

The interface operator N given in (14) consists of a nonlinear component driven by the function $\tilde{\mathbf{p}}(\mathbf{w})$ and a linear component. We characterise them by introducing the nonlinear function $\hat{\mathbf{p}}(\mathbf{w}) = \tilde{\mathbf{p}}(\mathbf{u}^1_h, \mathbf{u}^2_h) \otimes \mathbf{n}|_{\Omega^2}$ and the linear operator $L[\mathbf{w}] := -(\mathrm{I} - \mathrm{R})(\{W\mathbf{B}\}^{\upsilon} + \mathcal{B}_{\mathcal{J}}[\![\mathbf{w}]\!])$. Further, we abbreviate $\mathbb{S} := \mathbb{S}^1$, let $\mathbb{S}^*$ be the dual space of $\mathbb{S}$, and momentarily view N as an operator from $\mathbb{S} \to \mathbb{S}^*$, indicated with a calligraphic font:

$$\mathcal{N}:\ \mathbb{S} \to \mathbb{S}^*,\ \mathbf{w} \mapsto \Big(\mathbf{v} \mapsto \int_{\Gamma_{\mathcal{J}}} (\hat{\mathbf{p}}(\mathbf{w}) + L[\mathbf{w}]) : [\![\mathbf{v}]\!]\Big),$$

where the dependence on $\mathbf{v}$ represents a linear mapping $\mathbb{S} \to \mathbb{R}$ in $\mathbb{S}^*$. Thus the derivative $\mathcal{N}'$ is a mapping $\mathbb{S} \to L(\mathbb{S}, \mathbb{S}^*)$, where $L(\mathbb{S}, \mathbb{S}^*)$ denotes the linear mappings from $\mathbb{S}$ to $\mathbb{S}^*$. Therefore the integral

$$\mathcal{P}(t, \mathbf{v}) := \int_0^1 \mathcal{N}'(\mathbf{w}^\theta(t,\cdot))(\mathbf{v})\, d\theta,$$

where $\mathbf{w}^\theta := \theta\mathbf{u} + (1-\theta)\mathbf{w}_h$, belongs to $\mathbb{S}^*$ for each $t \in (0,T)$, $\mathbf{v} \in \mathbb{S}$. In particular $\mathcal{P}(t, \mathbf{u}(t,\cdot) - \mathbf{w}_h(t,\cdot)) \in \mathbb{S}^*$ and

$$\begin{aligned}\mathcal{P}(t, \mathbf{u}(t,\cdot) - \mathbf{w}_h(t,\cdot)) &= \int_0^1 \mathcal{N}'(\mathbf{w}^\theta(t,\cdot))(\mathbf{u}(t,\cdot) - \mathbf{w}_h(t,\cdot))\, d\theta \\ &= \int_0^1 \partial_\theta(\mathcal{N}(\mathbf{w}^\theta(t,\cdot)))\, d\theta = \mathcal{N}(\mathbf{u}(t,\cdot)) - \mathcal{N}(\mathbf{w}_h(t,\cdot)),\end{aligned} \tag{23}$$

using that $[0,1] \to \mathbb{S}^*$, $\theta \mapsto \mathcal{N}(\mathbf{w}^\theta(t,\cdot))$ is continuously differentiable as $\hat{\mathbf{p}} \in C^{1,1}(\mathbb{R}^{2n})$. We shall frequently abbreviate $\mathcal{P}(t, \mathbf{z}(t,\cdot))$ by $\mathcal{P}\mathbf{z}$ below.

We assume that there is an $s \in (3/2, 2]$ such that for all $\boldsymbol{\alpha} \in [L^2(\Omega)]^n$ and $\boldsymbol{\beta} \in [H^{1/2}(\Gamma_\mathcal{J})]^{2n}$ there exists a solution $\boldsymbol{\zeta} \in \mathbb{H}^s$ of the linear dual equation:

$$B(\mathbf{v}, \boldsymbol{\zeta}) + \lambda \langle \mathbf{v}, \boldsymbol{\zeta} \rangle + \langle \mathcal{P}\mathbf{v}, \boldsymbol{\zeta} \rangle = \langle \mathbf{v}, \boldsymbol{\alpha} \rangle + \langle \mathbf{v}, \boldsymbol{\beta} \rangle_{\Gamma_\mathcal{J}} \quad \forall\, \mathbf{v} \in \mathbb{H}^1, \tag{24}$$

satisfying

$$\sum_{j=1}^{2} \|\boldsymbol{\zeta}\|_{H^s(\Omega^j)} \lesssim \|\boldsymbol{\alpha}\| + \|\boldsymbol{\beta}\|_{H^{1/2}(\Gamma_\mathcal{J})}. \tag{25}$$

Lemma 5. *Assume that the hypothesis of Lemma 4 and* (24) *with* (25) *hold true. For $\lambda > 0$ sufficiently large, for $h_{\max}$ sufficiently small, the following error bound holds:*

$$\|\boldsymbol{\rho}\| \le C(1 + h_{\max}^2 \lambda)^{1/2} h_{\max}^{s-1} \, |||\boldsymbol{\eta}|||_{\mathcal{B},\lambda}. \tag{26}$$

If in addition the Hessian $\tilde{\mathbf{p}}''$ is uniformly bounded and $\mathbf{u}, \mathbf{u}_t \in W^{1,\infty}([0,T] \times \Gamma_\mathcal{J})$ then

$$\|\boldsymbol{\rho}_t\| \le C(1 + h_{\max}^2 \lambda)^{1/2} h_{\max}^{s-1} \, (|||\boldsymbol{\eta}_t|||_{\mathcal{B},\lambda} + |||\boldsymbol{\eta}|||_{\mathcal{B},\lambda}). \tag{27}$$

The constant C depends only on C_A and the shape-regularity of the mesh.

4. DG method for the parabolic system and its error analysis

The main contribution of this work is the derivation of optimal a priori bounds with substantially less restrictive assumptions on the reaction growth compared to the analysis presented in [11]. This will be done at the expense of introducing certain conditions on the mesh. This argument is motivated by ideas presented in [1, 19] for different problems.

To this end, consider $\mathbf{F}_L : \mathbb{R}^n \to \mathbb{R}^n$ satisfying

$$|\mathbf{F}_L(\mathbf{x}) - \mathbf{F}_L(\mathbf{y})| \le C_L |\mathbf{x} - \mathbf{y}|, \tag{28}$$

such that $\mathbf{F}(\mathbf{x}) = \mathbf{F}_L(\mathbf{x})$, for all $\mathbf{x} \in \mathbb{R}^n$ with $|\mathbf{x}| \le L := 2\max_{0 \le t \le T} \|\mathbf{u}(t)\|_\infty$. This implies, in particular, that $\mathbf{F}_L(\mathbf{u}) = \mathbf{F}(\mathbf{u})$.

Theorem 1. *Adopt the notation of Lemma 4 and the assumptions of Lemma 5. Assume also that $\mathbf{u} \in L^2(0,T;\mathbb{H}^s) \cap L^\infty(0, T \times \Omega)$, $s > 3/2$, $\mathbf{u}_t \in L^2(0,T;L^2(\Omega))$, $\mathbf{u}|_\kappa \in L^2(0,T;W^{2,\infty}(\kappa)) \cap H^1(0,T;[H^{k_\kappa+1}(\kappa)]^n)$, $k_\kappa \ge 1$, $\kappa \in \mathcal{T}$, and that the mesh $\mathcal{T}$ is fine enough so that*

$$h_{\min}^{-\frac{d}{2}} h_{\max}^{s-1} \mathcal{E}((0,T], \mathbf{h}, \mathbf{u}, \mathbb{V}_h) \tag{29}$$

is small enough with

$$\mathcal{E}((0,T], \mathbf{h}, \mathbf{u}, \mathbb{V}_h) := \Big(\sum_{\kappa \in \mathcal{T}} \int_0^T h_\kappa^{2s_\kappa} \big(|\mathbf{u}|^2_{[H^{s_\kappa+1}(\kappa)]^n} + |\mathbf{u}_t|^2_{[H^{s_\kappa+1}(\kappa)]^n} \big) \Big)^{1/2}, \tag{30}$$

for $s_\kappa = \min\{m_\kappa, k_\kappa\}$. Assume, finally, that $\mathbf{F}$ is locally Lipschitz. Then, we have

$$\|\mathbf{u} - \mathbf{u}_h\|_{L^\infty(0,T;L^2(\Omega))} \le C h_{\max}^{s-1} \mathcal{E}((0,T], \mathbf{h}, \mathbf{u}, \mathbb{V}_h), \tag{31}$$

with C independent of $\mathtt{h}$.

Proof. Assume initially that the locally Lipschitz continuous $\mathbf{F}$ is replaced with the globally Lipschitz continuous $\mathbf{F}_L$ from (28), and consider the modified initial/boundary value problem described in Section 2 with $\mathbf{F}$ replaced by $\mathbf{F}_L$. Noting that $\mathbf{F}_L(\mathbf{u}) = \mathbf{F}(\mathbf{u})$, we conclude that the analytical solution of the modified and of the original problem coincide. Let $\mathbf{u}_{Lh}$ denote the numerical solution of the modified problem by the dG method (12) with $\mathbf{F}$ replaced by $\mathbf{F}_L$.

Let $\mathbf{e}_L = \boldsymbol{\rho} + \boldsymbol{\theta}_L$, with $\boldsymbol{\rho} = \mathbf{u} - \mathbf{w}_h$ and $\boldsymbol{\theta}_L := \mathbf{w}_h - \mathbf{u}_{Lh}$. Orthogonality implies:

$$\langle (\mathbf{e}_L)_t, \boldsymbol{\theta}_L\rangle + B(\mathbf{e}_L, \boldsymbol{\theta}_L) + N(\mathbf{u}, \boldsymbol{\theta}_L) - N(\mathbf{u}_{Lh}, \boldsymbol{\theta}_L) + \langle \mathbf{F}(\mathbf{u}) - \mathbf{F}_L(\mathbf{u}_{Lh}), \boldsymbol{\theta}_L\rangle = 0.$$

Owing to (17), this gives

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\theta}_L\|^2 + B(\boldsymbol{\theta}_L, \boldsymbol{\theta}_L) = {}& \langle \mathbf{F}_L(\mathbf{u}_{Lh}) - \mathbf{F}(\mathbf{u}), \boldsymbol{\theta}_L\rangle \\ &+ N(\mathbf{u}_{Lh}, \boldsymbol{\theta}_L) - N(\mathbf{w}_h, \boldsymbol{\theta}_L) + \langle \lambda\boldsymbol{\rho} - \boldsymbol{\rho}_t, \boldsymbol{\theta}_L\rangle.\end{aligned} \tag{32}$$

Using the regularity of $\tilde{\mathbf{p}}$ and (11), we have

$$|N(\mathbf{u}_{Lh}, \boldsymbol{\theta}_L) - N(\mathbf{w}_h, \boldsymbol{\theta}_L)| \le C_{\mathcal{B}}^p \sum_{j=1}^{2} \|\boldsymbol{\theta}_L|_{\Omega^j}\|_{\Gamma_{\jmath}}^2 \le \frac{1}{4} C_{\mathrm{coer}} |||\boldsymbol{\theta}_L|||^2 + \frac{\lambda}{2}\|\boldsymbol{\theta}_L\|^2, \tag{33}$$

choosing ϵ and λ as in the proof of Lemma 4; we refer to [11] for details. The last term on the right-hand side of (32) can be treated as follows:

$$|\langle \lambda\boldsymbol{\rho} - \boldsymbol{\rho}_t, \boldsymbol{\theta}_L\rangle| \le \frac{\lambda}{2}\|\boldsymbol{\rho}\|^2 + \frac{1}{2\lambda}\|\boldsymbol{\rho}_t\|^2 + \lambda\|\boldsymbol{\theta}_L\|^2. \tag{34}$$

Since $\mathbf{F}_L(\mathbf{u}) = \mathbf{F}(\mathbf{u})$, the reaction term can be bounded as follows:

$$|\langle \mathbf{F}(\mathbf{u}) - \mathbf{F}_L(\mathbf{u}_{Lh}), \boldsymbol{\theta}_L\rangle| \le C_L \int_\Omega |\mathbf{u} - \mathbf{u}_{Lh}||\boldsymbol{\theta}_L| \le \frac{1}{2} C_L\big(\|\boldsymbol{\rho}\|^2 + 3\|\boldsymbol{\theta}_L\|^2\big). \tag{35}$$

Hence, (32) gives

$$\|\boldsymbol{\theta}_L(\tau)\|^2 + C_{\mathrm{coer}} \int_0^\tau |||\boldsymbol{\theta}_L|||^2 \le \delta_L^2 + 3(C_L + \lambda)\int_0^\tau \|\boldsymbol{\theta}_L\|^2, \tag{36}$$

with $\delta_L^2(t) = \int_0^T (C_L + \lambda)\|\boldsymbol{\rho}\|^2 + \lambda^{-1}\|\boldsymbol{\rho}_t\|^2 \mathrm{d}t$, noting that $\mathbf{u}_{Lh}(0) = \mathbf{u}_h(0)$. Gronwall's Lemma then implies

$$\|\boldsymbol{\theta}_L(\tau)\|^2 + C_{\mathrm{coer}} \int_0^\tau |||\boldsymbol{\theta}_L|||^2 \le \delta_L^2 \mathrm{e}^{3(C_L+\lambda)T}. \tag{37}$$

Hence the triangle inequality implies

$$\begin{aligned}\|\mathbf{e}_L\|_{L^\infty(0,T;L^2(\Omega))} &\le \delta_L \mathrm{e}^{3(C_L+\lambda)T/2} + \|\boldsymbol{\rho}\|_{L^\infty(0,T;L^2(\Omega))}\\ &\le C h_{\max}^{s-1}\mathcal{E}((0,T],\mathbf{h},\mathbf{u},\mathbb{V}_h),\end{aligned} \tag{38}$$

using Lemma 5 and standard L^2-projection approximation estimates.

We shall show that under the mesh assumption (29), the bound (38) also holds for $\mathbf{u}-\mathbf{u}_h$. To this end, consider the standard nodal interpolation operator $\mathcal{I}_\kappa : H^s(\kappa)\cap C(\bar{\kappa}) \to \mathbb{P}_{m_\kappa}$, (see, e.g., [14] for the scalar version), satisfying

$$|v-\mathcal{I}_\kappa v|_{H^j(\kappa)} \le C h_\kappa^{s-j}|v|_{H^s(\kappa)}, \tag{39}$$

for $0\le j\le s$ and $s\ge 2$, and

$$\|v-\mathcal{I}_\kappa v\|_{\infty,\kappa} \le C h_\kappa^2 |v|_{W^{2,\infty}(\kappa)}. \tag{40}$$

Let also $(\mathcal{I}v|_\kappa)_i := \mathcal{I}_\kappa v_i$, for $v=(v_1,\dots,v_n)\in[H^s(\kappa)\cap C(\bar{\kappa})]^n$. Then we have

$$\max_{0\le t\le T}\|\mathbf{u}_{Lh}\|_\infty \le \max_{0\le t\le T}\|\mathbf{u}_{Lh}-\mathcal{I}\mathbf{u}\|_\infty + \max_{0\le t\le T}\|\mathbf{u}-\mathcal{I}\mathbf{u}\|_\infty + \max_{0\le t\le T}\|\mathbf{u}\|_\infty. \tag{41}$$

The second and third terms on the right-hand side of (41) can be bounded using (40) and the definition of L, respectively, giving

$$\max_{0\le t\le T}\|\mathbf{u}_{Lh}\|_\infty \le \max_{0\le t\le T}\Big(\|\mathbf{u}_{Lh}-\mathcal{I}\mathbf{u}\|_\infty + C\Big(\sum_{\kappa\in\mathcal{T}} h_\kappa^4|\mathbf{u}|^2_{W^{2,\infty}(\kappa)}\Big)^{1/2}\Big) + \frac{L}{2}. \tag{42}$$

For the first term on the right-hand side of (42), a standard inverse estimate implies

$$\|\mathbf{u}_{Lh}-\mathcal{I}\mathbf{u}\|_\infty \le C\sum_{\kappa\in\mathcal{T}} h_\kappa^{-\frac{d}{2}}\|\mathbf{u}_{Lh}-\mathcal{I}\mathbf{u}\|_\kappa \le C\sum_{\kappa\in\mathcal{T}} h_\kappa^{-\frac{d}{2}}\big(\|\mathbf{e}_L\|_\kappa + \|\mathbf{u}-\mathcal{I}\mathbf{u}\|_\kappa\big).$$

Therefore, in view of (38) and (39), we deduce from (42) the bound

$$\max_{0\le t\le T}\|\mathbf{u}_{Lh}\|_\infty \le C h_{\min}^{-\frac{d}{2}} h_{\max}^{s-1}\mathcal{E}((0,T],\mathbf{h},\mathbf{u},\mathbb{V}_h) + C\Big(\sum_{\kappa\in\mathcal{T}} h_\kappa^4|\mathbf{u}|^2_{W^{2,\infty}(\kappa)}\Big)^{1/2} + \frac{L}{2}. \tag{43}$$

Choosing h such that the first two terms on the right-hand side of (43) are bounded strictly by $L/2$, one finds $\mathbf{u}_{Lh}=\mathbf{u}_h$, thereby concluding the proof. □

5. Error analysis for fully-discrete methods

We present an a priori error analysis for a simple fully discrete scheme consisting of the above dG method in space, together with simple implicit Euler time-stepping in time. To this end, we consider a subdivision $0=t_0<t_1<\dots<t_N=T$ of $[0,T]$, with local timestep $\tau_k := t_k - t_{k-1}$. The fully discrete scheme is defined as follows: for $k=1,2,\dots,N$, find $\mathbf{u}_h^k\in\mathbb{V}_h$ such that

$$\langle \partial\mathbf{u}_h^k,\mathbf{v}_h\rangle + B(\mathbf{u}_h^k,\mathbf{v}_h) + N(\mathbf{u}_h^k,\mathbf{v}_h) + \langle \mathbf{F}(\mathbf{u}_h^k),\mathbf{v}_h\rangle = 0,\quad \text{for all}\quad \mathbf{v}_h\in\mathbb{V}_h, \tag{44}$$

with $\partial \mathbf{u}_h^k := (\mathbf{u}_h^k - \mathbf{u}_h^{k-1})/\tau_k$.

Setting $\mathbf{e}^k := \mathbf{u}^k - \mathbf{u}_h^k = \boldsymbol{\rho}^k + \boldsymbol{\theta}^k$ with $\boldsymbol{\rho}^k := \mathbf{u}^k - \mathbf{w}_h^k$ and $\boldsymbol{\theta}^k := \mathbf{w}_h^k - \mathbf{u}_h^k$, where $\mathbf{u}^k = \mathbf{u}(t_k)$ the exact solution to the PDE system (1)–(6) at time t_k, and $\mathbf{w}_h^k \in \mathbb{V}_h$ is given by

$$B(\mathbf{u}^k - \mathbf{w}_h^k, \mathbf{v}_h) + N(\mathbf{u}^k, \mathbf{v}_h) - N(\mathbf{w}_h^k, \mathbf{v}_h) + \lambda \langle \mathbf{u}^k - \mathbf{w}_h^k, \mathbf{v}_h \rangle = 0 \quad \forall \mathbf{v}_h \in \mathbb{V}_h, \tag{45}$$

for $\lambda > 0$.

Theorem 2. *Adopt the notation of Lemma 4 and the assumptions of Lemma 5. Assume also that* $\mathbf{u} \in L^2(0,T;\mathbb{H}^s) \cap L^\infty([0,T] \times \Omega)$*,* $s > 3/2$*,* $\mathbf{u}_t, \mathbf{u}_{tt} \in L^2(0,T;L^2(\Omega))$*,* $\mathbf{u}|_\kappa \in L^2(0,T;W^{2,\infty}(\kappa)) \cap H^1(0,T;[H^{k_\kappa+1}(\kappa)]^n)$*,* $k_\kappa \geq 1$*,* $\kappa \in \mathcal{T}$*, and that the space and time meshes are fine enough so that*

$$h_{\min}^{-\frac{d}{2}} \Big(h_{\max}^{s-1} \mathcal{E}^N(\mathbf{h}, \mathbf{u}, \mathbb{V}_h) + \sum_{q=1}^{k} \tau_q^2 \int_{t^{q-1}}^{t^q} \|\mathbf{u}_{tt}\| \Big) \tag{46}$$

is small enough, with

$$\mathcal{E}^k(\mathbf{h}, \mathbf{u}, \mathbb{V}_h) := \Big(\sum_{q=1}^{k} \tau_k \Big(\sum_{\kappa \in \mathcal{T}} h_\kappa^{2s_\kappa} \big(|\mathbf{u}|^2_{[H^{s_\kappa+1}(\kappa)]^n} + |\mathbf{u}_t|^2_{[H^{s_\kappa+1}(\kappa)]^n} \big) \Big) \Big)^{1/2}, \tag{47}$$

for $s_\kappa = \min\{m_\kappa, k_\kappa\}$*,* $k = 1, \dots, N$*. Assume, finally, that* $\mathbf{F}$ *is locally Lipschitz. Then, we have*

$$\max_{0 \leq k \leq N} \|\mathbf{u}^k - \mathbf{u}_h^k\| \leq C \Big(h_{\max}^{s-1} \mathcal{E}^N(\mathbf{h}, \mathbf{u}, \mathbb{V}_h) + \sum_{q=1}^{k} \tau_q^2 \int_{t^{q-1}}^{t^q} \|\mathbf{u}_{tt}\| \Big). \tag{48}$$

Proof. As before, assume for the moment that $\mathbf{F} : \mathbb{R}^n \to \mathbb{R}^n$ is replaced by $\mathbf{F}_L$ described above and let $\mathbf{u}_{Lh}^k$ denote the numerical solution of the modified problem by the dG method given by (44) with $\mathbf{F}$ replaced by $\mathbf{F}_L$.

Setting $\mathbf{e}_L^k = \boldsymbol{\rho}^k + \boldsymbol{\theta}_L^k$, with $\boldsymbol{\theta}_L^k := \mathbf{w}_h^k - \mathbf{u}_{Lh}^k \in \mathbb{V}_h$, and $\mathbf{w}_h^k$ as above, Galerkin orthogonality implies:

$$\langle \mathbf{u}_t^k - \partial \mathbf{u}_{Lh}^k, \boldsymbol{\theta}_L^k \rangle + B(\mathbf{e}_L^k, \boldsymbol{\theta}^k) + N(\mathbf{u}^k, \boldsymbol{\theta}_L^k) - N(\mathbf{u}_{Lh}^k, \boldsymbol{\theta}_L^k) + \langle \mathbf{F}(\mathbf{u}^k) - \mathbf{F}_L(\mathbf{u}_{Lh}^k), \boldsymbol{\theta}_L^k \rangle = 0.$$

Using (45), this gives

$$\begin{aligned} \langle \partial \boldsymbol{\theta}_L^k, \boldsymbol{\theta}_L^k \rangle + B(\boldsymbol{\theta}_L^k, \boldsymbol{\theta}_L^k) = {}& \langle \mathbf{F}_L(\mathbf{u}_{Lh}^k) - \mathbf{F}(\mathbf{u}^k), \boldsymbol{\theta}_L^k \rangle + N(\mathbf{u}_{Lh}^k, \boldsymbol{\theta}_L^k) - N(\mathbf{w}_h^k, \boldsymbol{\theta}_L^k) \\ & + \langle \lambda \boldsymbol{\rho}^k - \partial \boldsymbol{\rho}^k + \partial \mathbf{u}^k - \mathbf{u}_t^k, \boldsymbol{\theta}_L^k \rangle. \end{aligned} \tag{49}$$

The terms involving the semilinear form $N(\cdot,\cdot)$ can be bounded in a completely analogous fashion to (33), while the last term on the right-hand side of (49) can be bounded as follows:

$$|\langle \lambda \boldsymbol{\rho}^k - \partial \boldsymbol{\rho}^k + \partial \mathbf{u}^k - \mathbf{u}_t^k, \boldsymbol{\theta}_L^k \rangle| \leq \frac{\lambda}{2} \|\boldsymbol{\rho}^k\|^2 + \frac{1}{2\lambda} (\|\partial \boldsymbol{\rho}^k\| + \|\partial \mathbf{u}^k - \mathbf{u}_t^k\|)^2 + \lambda \|\boldsymbol{\theta}_L^k\|^2. \tag{50}$$

Since $\mathbf{F}_L(\mathbf{u}) = \mathbf{F}(\mathbf{u})$, for all $t \in [0,T]$, for the nonlinear reaction term we have:

$$|\langle \mathbf{F}(\mathbf{u}^k) - \mathbf{F}_L(\mathbf{u}^k_{Lh}), \boldsymbol{\theta}^k_L\rangle| \leq C_L \int_\Omega |\mathbf{u}^k - \mathbf{u}^k_{Lh}||\boldsymbol{\theta}^k_L| \leq \frac{1}{2} C_L\big(\|\boldsymbol{\rho}^k\|^2 + 3\|\boldsymbol{\theta}^k_L\|^2\big). \quad (51)$$

Hence, (49) gives

$$\|\boldsymbol{\theta}^k_L\|^2 + C_{\rm coer}\sum_{q=1}^{k} \tau_k |||\boldsymbol{\theta}^q_L|||^2 \leq (\delta^k_L)^2 + 3(C_L+\lambda)\sum_{q=1}^{k}\tau_k\|\boldsymbol{\theta}^q_L\|^2, \quad (52)$$

where

$$(\delta^k_L)^2 = (C_L+\lambda)\sum_{q=1}^{k}\tau_q\Big(\|\boldsymbol{\rho}^q\|^2 + \lambda^{-1}(\|\partial\boldsymbol{\rho}^q\| + \|\partial\mathbf{u}^q - \mathbf{u}^q_t\|)^2\Big) + \|\boldsymbol{\theta}^0\|^2, \quad (53)$$

noting that $\mathbf{u}^0_{Lh} = \mathbf{u}^0_h$. The discrete version of Gronwall's Lemma implies

$$\|\boldsymbol{\theta}^k_L\|^2 + C_{\rm coer}\sum_{q=1}^{k}\tau_q|||\boldsymbol{\theta}^q_L|||^2 \leq (\delta^k_L)^2 \mathrm{e}^{3(C_L+\lambda)T}. \quad (54)$$

Using the triangle inequality, we arrive at

$$\max_{1\leq k\leq N}\|\mathbf{e}^k_L\|^2 \leq \max_{1\leq k\leq N}((\delta^k_L)^2\mathrm{e}^{3(C_L+\lambda)T} + \|\boldsymbol{\rho}^k\|^2). \quad (55)$$

To show that the right-hand side of (55) converges optimally with respect to the local mesh-size and with respect to the time-step, we work as follows. We begin by setting $t = t^k$, $\mathbf{v} = \boldsymbol{\rho}^k$ $\boldsymbol{\alpha} = \partial\boldsymbol{\rho}^k$, $\boldsymbol{\beta} = \mathbf{0}$, and $t = t^{k-1}$, $\mathbf{v} = \boldsymbol{\rho}^{k-1}$ $\boldsymbol{\alpha} = \partial\boldsymbol{\rho}^k$, $\boldsymbol{\beta} = \mathbf{0}$ on (24), respectively, with exact (dual) solutions $\mathbf{z}^k$ and $\mathbf{z}^{k-1}$, respectively, and we use the resulting equations to arrive at

$$\begin{aligned}
\tau_k\|\partial\boldsymbol{\rho}^k\|^2 &= \langle \boldsymbol{\rho}^k - \boldsymbol{\rho}^{k-1}, \partial\boldsymbol{\rho}^k\rangle \\
&= B(\boldsymbol{\rho}^k,\mathbf{z}^k) + \lambda\langle\boldsymbol{\rho}^k,\mathbf{z}^k\rangle + N(\mathbf{u}^k,\mathbf{z}^k) - N(\mathbf{w}^k,\mathbf{z}^k) \\
&\quad - B(\boldsymbol{\rho}^{k-1},\mathbf{z}^{k-1}) - \lambda\langle\boldsymbol{\rho}^{k-1},\mathbf{z}^{k-1}\rangle - N(\mathbf{u}^{k-1},\mathbf{z}^{k-1}) + N(\mathbf{w}^{k-1},\mathbf{z}^{k-1}) \\
&= B(\boldsymbol{\rho}^k,\boldsymbol{\eta}_{\mathbf{Z}^k}) + \lambda\langle\boldsymbol{\rho}^k,\boldsymbol{\eta}_{\mathbf{Z}^k}\rangle + N(\mathbf{u}^k,\boldsymbol{\eta}_{\mathbf{Z}^k}) - N(\mathbf{w}^k,\boldsymbol{\eta}_{\mathbf{Z}^k}) \\
&\quad - B(\boldsymbol{\rho}^{k-1},\boldsymbol{\eta}_{\mathbf{Z}^{k-1}}) - \lambda\langle\boldsymbol{\rho}^{k-1},\boldsymbol{\eta}_{\mathbf{Z}^{k-1}}\rangle - N(\mathbf{u}^{k-1},\boldsymbol{\eta}_{\mathbf{Z}^{k-1}}) + N(\mathbf{w}^{k-1},\boldsymbol{\eta}_{\mathbf{Z}^{k-1}}),
\end{aligned} \quad (56)$$

with $\boldsymbol{\eta}_{\mathbf{Z}^k} := \mathbf{z}^k - \Pi\mathbf{z}^k$, $k = 1,\dots,N$, where in the last equality we used the definition of the elliptic projection (45). Using continuity of the bilinear form, the piecewise trace inequality discussed above, along with standard approximation estimates, one can show

$$\tau_k\|\partial\boldsymbol{\rho}^k\|^2 \leq Ch^{2s-2}_{\max}\sum_{\kappa\in\mathcal{T}} h^{2s_\kappa}_\kappa |\mathbf{u}|^2_{[H^{s_\kappa+1}(\kappa)]^n};$$

the details are omitted here for brevity (see the proof of Lemma 4.5 in [11] for details). Also, $\|\partial\mathbf{u}^q - \mathbf{u}^q_t\|$, can be bounded straightforwardly using the integral form of Taylor expansion. The rest of the terms in δ_L^k as in the proof of Lemma 3.6. This line of argument results to the bound

$$\max_{1\le k\le N}\|\mathbf{e}_L^k\| \le (\delta_L^k)^2 e^{\frac{3}{2}(C_L+\lambda)T}+\|\boldsymbol{\rho}^k\| \le Ch_{\max}^{s-1}\Big(\mathcal{E}^N(\mathbf{h},\mathbf{u},\mathbb{V}_h)+\sum_{q=1}^{k}\tau_q^2\int_{t^{q-1}}^{t^q}\|\mathbf{u}_{tt}\|\Big),$$

whose right-hand side becomes arbitrarily small, for sufficiently small $h_{\max}$ and $\max_{q=1,\dots,k}\tau_q$.

We shall now show that, provided (46) is sufficiently small, the same bound also holds for the dG method of the original problem. To this end, we have

$$\max_{1\le k\le N}\|\mathbf{u}_{Lh}^k\|_\infty \le \max_{1\le k\le N}\big(\|\mathbf{u}_{Lh}^k-\mathfrak{I}\mathbf{u}^k\|_\infty+\|\mathbf{u}^k-\mathfrak{I}\mathbf{u}^k\|_\infty+\|\mathbf{u}^k\|_\infty\big).$$

For the second and third terms on the right-hand side of the above bound, we use (40) and the definition of L, respectively, giving

$$\max_{1\le k\le N}\|\mathbf{u}_{Lh}^k\|_\infty \le \max_{1\le k\le N}\Big(\|\mathbf{u}_{Lh}^k-\mathfrak{I}\mathbf{u}^k\|_\infty+C\Big(\sum_{\kappa\in\mathfrak{T}}h_\kappa^4|\mathbf{u}^k|^2_{W^{2,\infty}(\kappa)}\Big)^{1/2}\Big)+\frac{L}{2}. \tag{57}$$

As before, the first term on the right-hand side of the above bound can be bounded using a standard inverse estimate, viz.,

$$\|\mathbf{u}_{Lh}^k-\mathfrak{I}\mathbf{u}^k\|_\infty \le C\sum_{\kappa\in\mathfrak{T}}h_\kappa^{-\frac{d}{2}}\|\mathbf{u}_{Lh}^k-\mathfrak{I}\mathbf{u}^k\|_\kappa \le C\sum_{\kappa\in\mathfrak{T}}h_\kappa^{-\frac{d}{2}}\big(\|\mathbf{e}_L^k\|_\kappa+\|\mathbf{u}^k-\mathfrak{I}\mathbf{u}^k\|_\kappa\big).$$

Therefore, in view of (38) and (39), we deduce the bound

$$\begin{aligned}\max_{0\le k\le N}\|\mathbf{u}_{Lh}^k\|_\infty \le{}& Ch_{\min}^{-\frac{d}{2}}h_{\max}^{s-1}\Big(\mathcal{E}^N(\mathbf{h},\mathbf{u},\mathbb{V}_h)+\sum_{q=1}^{k}\tau_q^2\int_{t^{q-1}}^{t^q}\|\mathbf{u}_{tt}\|\Big)\\ &+C\max_{1\le k\le N}\Big(\sum_{\kappa\in\mathfrak{T}}h_\kappa^4|\mathbf{u}^k|^2_{W^{2,\infty}(\kappa)}\Big)^{1/2}+\frac{L}{2}.\end{aligned} \tag{58}$$

Choosing $h_{\max}$ small enough, at least small enough so that (46) is sufficiently small, the first two terms on the right-hand side of (58) are dominated by $L/2$, which then already implies that $\mathbf{u}_{Lh}=\mathbf{u}_h$, thereby concluding the proof. □

6. Numerical examples

To highlight the practicality of the fully discrete scheme, we present here a numerical experiment with cubic reactions; for a numerical convergence study of the spatial discretization with a known exact solution we refer to [11].

We set $\Omega=[-1,1]^2$, with $\Omega^1=[-1,0]\times[-1,1]$ and $\Omega^2=[0,1]\times[-1,1]$, so that $\Gamma_{\mathfrak{I}}=\{0\}\times(-1,1)$. We set $\Gamma_{\mathrm{N}}=\partial\Omega$. For $t>0$ we consider a system of two advection-diffusion equations (1), (2), (4), (5), (6) with $a_1=a_2=.1$, $B_1=B_2=(-1,-1)$, and

$$\mathbf{F}(\mathbf{u})=\begin{pmatrix}-u_1^3+u_1u_2\\ u_1^3-u_1u_2\end{pmatrix}. \tag{59}$$

We set $\mathbf{g}_{\mathrm{N}} = \mathbf{0}$ and fix the flux function (7) with $\tilde{\mathbf{p}} = u_2 - u_1$, $\Upsilon^1 = \mathrm{diag}(.4, .4)$, $\Upsilon^2 = \mathrm{diag}(.6, .6)$, and $\mathrm{R} = \mathrm{diag}(1, 1)$. The initial condition is

$$u_1|_{\Omega^1} = 0, \quad u_1|_{\Omega^2} = e^{(y^2-1)^2}(-4x^3 + 3x + 1), \quad u_2|_{\Omega^1} = u_2|_{\Omega^2} = 0.$$

The computational domain is subdivided using a uniform 64×64 mesh. The time step is $k = 10^{-2}$. We solve the problem using the fully implicit method described and analysed in the previous sections using bilinear elements. Few snapshots of the numerical solution are shown in Figure 2. Both components of the solution are discontinuous at the interface. Although no exact solution is available, the numerical solution appears to be stable and convergent, when compared to numerical solutions on different meshes. The `deal.ii` library was used for the above numerical experiments.

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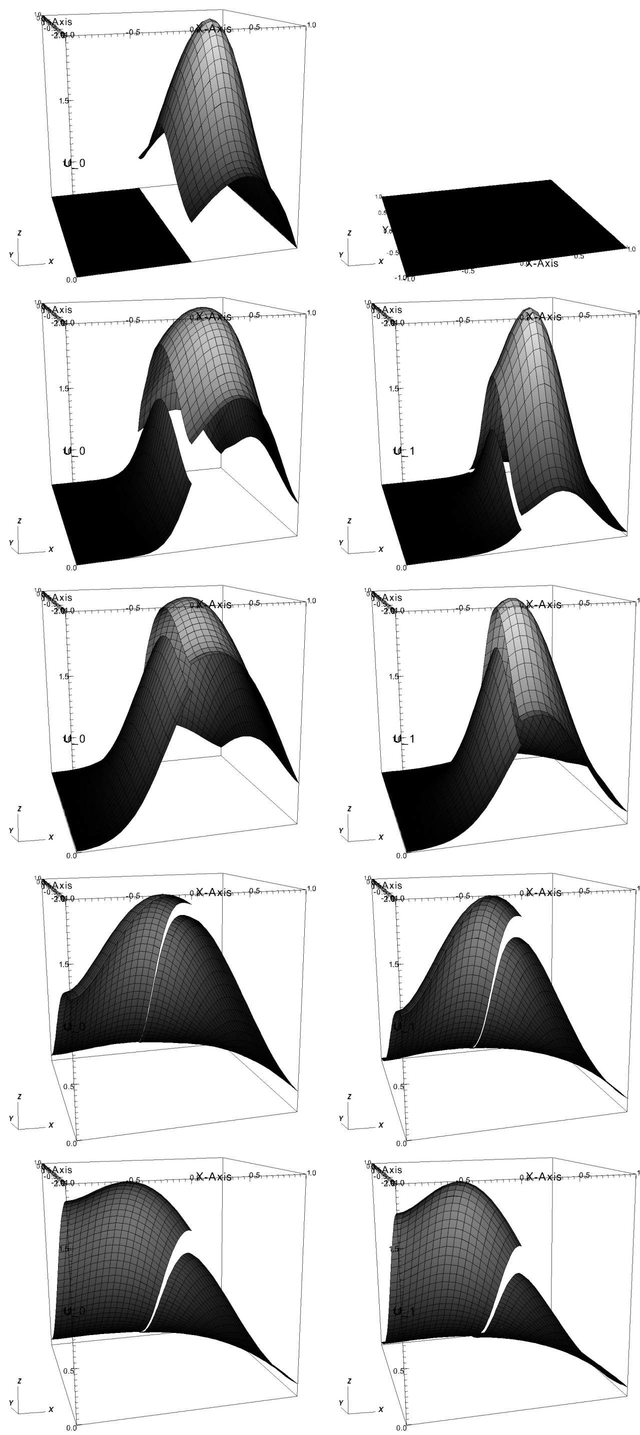

Figure 2: Numerical test. Snapshots of the solution u_1 (left) and u_2 (right) computed on a uniform 64×64 mesh using bilinear elements: the initial condition (top) followed by the solution at times $t = .05, .25, .75, 1$.

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