DISCONTINUOUS GALERKIN METHODS FOR CONVECTION-DIFFUSION PROBLEMS MODELLING MASS-TRANSFER THROUGH SEMIPERMEABLE MEMBRANES

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Abstract. We propose a family of Interior Penalty Discontinuous Galerkin (IP-DG) finite element methods for the solution of semilinear convection-reaction-diffusion systems on partitioned subdomains arising in the modelling of mass transfer through semipermeable membranes. Non-linear interface conditions are imposed at the sub-domain interfaces. The problem considered is relevant to the modelling of chemical species passing through thin biological membranes. In particular, we consider applications in cellular signal transduction. A series of numerical experiments highlight the good stability and accuracy properties of the proposed method.
1 INTRODUCTION
This work proposes the use of interior-penalty discontinuous Galerkin finite element methods to non-linear convection-diffusion-reaction interface problems with non-linear coupling conditions, imposed along an interface cutting through the solution domain. The method is derived under the assumption that the finite element mesh is aligned with the interfaces and choosing appropriate numerical fluxes at the inter-element boundaries.

This setting is motivated by problems of mass-transfer of a number of substances (solutes) through semi-permeable membranes [7]. The interface conditions considered include well established models of thin biological membranes [10, 9] and of mass transfer models for the solution of solute dynamics across arterial walls [12].

In their first decades of development, Discontinuous Galerkin (DG) finite element methods have been analysed independently for the solution of problems with discontinuous solutions, with their introduction in the context of first-order hyperbolic problems due to Reed and Hill [13], and for the solution of parabolic and elliptic problems, with the introduction of the methods generally referred to as penalty methods [11, 3, 4, 15, 2].

The Discontinuous Galerkin approach offers a number of advantages in the numerical simulation. First, due to being discontinuous across element interfaces, DG methods permit the imposition of the interface conditions in a very natural way. Moreover, they are ideally suited for the solution of problems of mixed type (i.e., problems where the diffusion may be degenerate or absent in parts of the computational domain) [8]. Furthermore, discontinuous Galerkin methods are well suited to time-dependent problems as they yield block diagonal mass matrices that can be inverted easily. This is because the local elemental bases can be chosen freely due to the lack of any conformity requirement across the element interfaces. This implies that there is no need for mass-lumping which can be problematic when using high-order finite element bases.

The rest of this work is structured as follows. In Section 2 we describe the system of partial differential equations (PDE) along with the respective initial, boundary and interface conditions under consideration. In Section 3 we present the new interior-penalty discontinuous Galerkin method for the class of PDE systems described in Section 2. Section 4 contains a series of numerical experiments indicating the good performance of the proposed numerical method. Finally, in Section 5, we draw some conclusions.

2 MODEL PROBLEM AND NOTATION
Let \( \Omega \) be a bounded open computational domain with Lipschitz boundary in \( \mathbb{R}^d \), and let \( \partial \Omega \) be the boundary of \( \Omega \). The domain \( \Omega \) is split into two subdomains \( \Omega_1 \) and \( \Omega_2 \), such that \( \Omega = \Omega_1 \cup \Omega_2 \cup \Gamma_{\text{tr}} \), where \( \Gamma_{\text{tr}} := \overline{\Omega_1} \cap \overline{\Omega_2} \) and \( \Omega_1 \) (and, therefore, \( \Omega_2 \) also) have Lipschitz boundaries, see, e.g., Figure 1 for an illustration.

We also define \( \mathcal{H}^1 := [H^1(\Omega_1 \cup \Omega_2)]^n \), where \( H^1(\Omega_1 \cup \Omega_2) \) signifies the space of square integrable functions on \( \Omega_1 \cup \Omega_2 \) with square integrable (weak) derivative. For a vector function \( \mathbf{v} : \Omega_1 \cup \Omega_2 \to \mathbb{R}^n \) with \( \mathbf{v} \in \mathcal{H}^1 \), we define its gradient \( \nabla \mathbf{v} : \Omega_1 \cup \Omega_2 \to \mathbb{R}^{n \times d} \).
by \( \nabla v := (\nabla v_1, \ldots, \nabla v_n)^T \), with \( \nabla v_i(x) \in \mathbb{R}^d \), \( i = 1, \ldots, n \), \( x \in \Omega_1 \cup \Omega_2 \). Further, for a tensor \( Q : \Omega_1 \cup \Omega_2 \to \mathbb{R}^{nxd} \), with rows \( Q_i \), \( i = 1, \ldots, n \), we define its divergence
\[
\nabla \cdot Q := (\nabla \cdot Q_1, \ldots, \nabla \cdot Q_n)^T.
\]

For a time interval \([0, T]\), \( T > 0 \), and for \( u := (u_1, \ldots, u_n)^T \), we consider the system of semilinear equations
\[
u_t - \nabla \cdot (A \nabla u - UB) + F(u) = 0 \quad \text{in } [0, T] \times (\Omega_1 \cup \Omega_2),
\]
for a vector field \( F : \mathbb{R}^n \to \mathbb{R}^n \) and for \( n \times d \)-matrix \( B \), whose rows are denoted by \( B_i \), \( i = 1, \ldots, n \), and \( A \) an \( n \times n \) diagonal matrix, with \( A = (a_{12}, \ldots, a_{nn}) \), where \( a_i : (0, T] \times \Omega \to \mathbb{R} \), \( i = 1, \ldots, n \), and for diagonal matrix with \( U = (u_1, \ldots, u_n) \). We assume that \( a_i > 0 \), for all \( i = 1, \ldots, n \). We shall also make use of the \( n \times n \)-matrix \( D \) defined by \( D := 1/2(\nabla \cdot B_1, \ldots, \nabla \cdot B_n) \); \( B \) is assumed to be so as to make \( D \) positive semi-definite.

We impose the initial condition
\[
u(0, x) = \nu_0(x) \quad \text{on } \{0\} \times \Omega,
\]
for some initial condition vector \( \nu_0 \). On \([0, T] \times \partial \Omega \), we impose mixed Dirichlet and Neumann boundary conditions as follows. For \( i = 1, \ldots, n \), the boundary \( \partial \Omega \) is split into \( \partial \Omega = \partial_D \cup \partial_N \), with \( \partial_D \) being of positive \((d - 1)\)-dimensional (Hausdorff) measure. Further, for \( i = 1, \ldots, n \), we subdivide \( \partial \Omega = \partial \Omega_i - \partial \Omega_i^+ \), where \( \partial \Omega_i^+ := \{ x \in \partial \Omega : (B_i \cdot n)(x) < 0 \} \) and \( \partial \Omega_i^+ = \partial \Omega \setminus \partial \Omega_i^- \), the inflow and outflow parts of the boundary \( \partial \Omega \) for the \( i \)-th equation. For \( i = 1, \ldots, n \), we assign
\[
\begin{align*}
u_i = g_D^i & \quad \text{on } \partial_D, \\
(a_i \nabla u_i - B_i \nu_i) \cdot n = g_N^i & \quad \text{on } \partial_D \cap \partial \Omega_i^+, \\
(a_i \nabla u_i - B_i \nu_i) \cdot n = g_N^i & \quad \text{on } \partial_D \cap \partial \Omega_i^-, 
\end{align*}
\]
for Dirichlet and Neumann data \( g_D, g_N \), respectively; \( n \in \mathbb{R}^d \) denotes the unit outward normal vector to \( \partial \Omega \). We denote by \( \chi^- : \partial \Omega_i^- \to \mathbb{R} \), the characteristic function of \( \partial \Omega_i^- \), and by \( \chi^+ := 1 - \chi^- \), i.e., the characteristic function of \( \partial \Omega_i^+ \). Abusing the notation, we shall collectively refer to these quantities by \( \chi^- \) and \( \chi^+ \), respectively, and we shall frequently write (3) as
\[
u = g_D \quad \text{on } \partial_D \quad \text{and} \quad (A \nabla u - \chi^- U B) n = g_N \quad \text{on } \partial_N,
\]
where \( g_D := (g_{D1}, \ldots, g_{Dn})^T \) and \( g_N := (g_{N1}, \ldots, g_{Nn})^T \). Interface conditions are imposed across \( \Gamma_{tr} \), reading
\[
\begin{align*}
(a_i \nabla u_i - u_i B_i) \cdot n|_{\Gamma_1} = p_1 (u^1, u^2) (u_i|_{\Gamma_1} - u_i|_{\Gamma_2}) - (\zeta^1_i u_i|_{\Gamma_1} + \zeta^2_i u_i|_{\Gamma_2})(B_i \cdot n)|_{\Gamma_1}, & \quad \text{on } \Gamma_{tr}, \\
(a_i \nabla u_i - u_i B_i) \cdot n|_{\Gamma_2} = p_2 (u^1, u^2) (u_i|_{\Gamma_2} - u_i|_{\Gamma_1}) - (\zeta^1_i u_i|_{\Gamma_1} + \zeta^2_i u_i|_{\Gamma_2})(B_i \cdot n)|_{\Gamma_2}, & \quad \text{on } \Gamma_{tr},
\end{align*}
\]

\( p_1, p_2 \) are positive semi-definite.
where $u^j := u|_{\Omega_j \cap \Gamma_{tr}}$, $j = 1, 2$, and $n|_{\partial e}$ denotes the unit outward normal vector to $\Gamma_{tr}$ from $\Omega_j$, $j = 1, 2$. The above interface conditions are written in terms of the weights $\zeta_{\kappa}^{i,2} \in [0,1]$ and permeabilities $p_i : [\Gamma_{tr}]^2 \to \mathbb{R}$, $i = 1, \ldots, n$. The weights $\zeta_{\kappa}^{i,2}$ are such that $\zeta_{\kappa}^{i} + \zeta_{\kappa}^{i,2} = 1$ and $\zeta_{\kappa}^{i} \geq \zeta_{\kappa}^{i,2}$ if $(B_i \cdot n)|_{\Omega_i} \geq 0$ on $\Gamma_{tr}$. Further, the permeabilities $p_i$ are assumed to be Lipschitz continuous with Lipschitz continuous total derivatives. It is by all means possible in the results described below to consider a different interface manifold $\Gamma_{tr}$ for each equation, as well as to split $\Omega$ in more than two subregions. We refrain from doing so, in the interest of simplicity of the presentation only. Finally, we assume that $\mathbf{F}$ satisfies a locally Lipschitz growth condition.

### 3 DISCONTINUOUS GALERKIN FINITE ELEMENT METHOD

Let $\mathcal{T}$ be a shape-regular subdivision of $\Omega$ into disjoint open elements $\kappa \in \mathcal{T}$, such that $\Gamma_{tr} \subset \cup_{\kappa \in \mathcal{T}} \partial \kappa =: \Gamma$, the skeleton. Further we decompose $\Gamma$ into three disjoint subsets $\Gamma = \partial \Omega \cup \Gamma_{int} \cup \Gamma_{tr}$, where $\Gamma_{int} := \Gamma \setminus (\partial \Omega \cup \Gamma_{tr})$. We assume that the subdivision $\mathcal{T}$ is constructed via mappings $F_\kappa$, 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; the maps are assumed to be constructed so as to ensure that the union of the closures of the elements $\kappa \in \mathcal{T}$ forms a covering of the closure of $\Omega$, i.e., $\overline{\Omega} = \cup_{\kappa \in \mathcal{T}} \overline{\kappa}$.

For a nonnegative integer $m$, we denote by $\mathcal{P}_{m}(\hat{\kappa})$, the set of polynomials of total degree at most $m$ if $\hat{\kappa}$ is the reference simplex, or the set of all tensor-product polynomials on $\hat{\kappa}$ of degree $m$ in each variable, if $\hat{\kappa}$ is the reference hypercube. We consider the discontinuous finite element space

$$s := \{v \in L^2(\Omega) : v|_{\kappa} \circ F_\kappa \in \mathcal{P}_{m}(\hat{\kappa}), \kappa \in \mathcal{T}\},$$

and set $S := [s]^n$.

Next, we introduce some trace operators. Let $\kappa^+, \kappa^-$ be two (generic) elements sharing an edge $e := \partial \kappa^+ \cap \partial \kappa^- \subset \Gamma_{int} \cup \Gamma_{tr}$. Define the outward normal unit vectors $n^+$ and $n^-$ on $e$ corresponding to $\partial \kappa^+$ and $\partial \kappa^-$, respectively. For functions $q : \Omega \to \mathbb{R}^n$ and $Q : \Omega \to \mathbb{R}^{n \times d}$ that may be discontinuous across $\Gamma$, we define the following quantities. For $q^+ := q|_{e \subset \partial \kappa^+}$, $q^- := q|_{e \subset \partial \kappa^-}$, and $Q^+ := Q|_{e \subset \partial \kappa^+}$, $Q^- := Q|_{e \subset \partial \kappa^-}$, we set

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

and

$$[q] := q^+ \otimes n^+ + q^- \otimes n^-, \quad [Q] := Q^+ n^+ + Q^- n^-,$$

where $\otimes$ denotes the standard tensor product operator, whereby $q \otimes w = qw^T$; if $e \in \partial \kappa \cap \partial \Omega$, these definitions are modified as follows

$$\{q\} := q^+, \quad \{Q\} := Q^+, \quad [q] := q^+ \otimes n, \quad [Q] := Q^+ n.$$
Finally, we introduce the mesh quantities \( h : \Omega \to \mathbb{R}, m : \Omega \to \mathbb{R} \), by \( h(x) = \text{diam} \kappa, m(x) = m_\kappa \), if \( x \in \kappa \), and \( h(x) = \{ h \}, m(x) = \{ m \} \), if \( x \in \Gamma \), respectively.

We are now ready to describe the (symmetric) \textit{interior penalty discontinuous Galerkin method} the PDE system from Section 2: find \( w_h \in S \) such that for \( t \in (0, T_f] \), find \( u_h \equiv u_h(t) \in S \) such that

\[
\langle (u_h)_t, v_h \rangle + B(u_h, v_h) + N(u_h, v_h) + \langle F(u_h), v_h \rangle = 0, \quad \text{for all } v_h \in S. \tag{7}
\]

where \( \langle u, v \rangle := \int_{\Omega} uv dx \),

\[
B(w_h, v_h) = \sum_{\kappa \in T_h} \int_{\kappa} (A \nabla w_h - W_B) : \nabla v_h + \int_{\Gamma} (\{ W_B \} + \mathbb{B}_{tr}[w_h]) : \|v_h\| \\
- \int_{\Gamma_D} (A \nabla w_h - \chi^\kappa W_B) : (v_h \otimes n) + (A \nabla v_h) : (w_h \otimes n) - \Sigma w_h \cdot v_h \\
- \int_{\Gamma_{in}} (A \nabla w_h - W_B) : \|v_h\| + \{ A \nabla v_h \} : \|w_h\| - (\Sigma + \mathbb{B})[w_h] : \|v_h\| \tag{8}
\]

and

\[
N(w_h, v_h) := \int_{\Gamma_{tr}} P(w_h)[w_h] : \|v_h\|, \tag{9}
\]

for \( w \in S \), and

\[
l(v_h) := \int_{\Gamma_D} (- (g_D \otimes n) : (A \nabla v_h) - (\chi^- G_D B) : (v_h \otimes n) + \Sigma g_D \cdot v_h) + \int_{\Gamma_N} g_N \cdot v_h, \tag{10}
\]

noting that \((q \otimes n) : (v \otimes n) = q \cdot v \), for \( q, v \in \mathbb{R}^n \). In this setting, \( \Gamma_N \) can have non-trivial intersection with both \( \partial \Omega^- \) and \( \partial \Omega^+ \), thereby extending the discontinuous Galerkin method proposed in [8]. We note that the method is carefully constructed to yield stable discretisations even in the challenging case of convection-dominated flows.

4 NUMERICAL EXPERIMENTS

We introduce a fully discrete discretisation for the PDE system from Section 2 using an implicit-explicit discretisation [6, 1] (implicit in the linear part of the differential operator and explicit in the nonlinear parts).

Our first numerical example is set up on the square domain \( \Omega = [-1, 1]^2 \) subdivided into two subdomains interfacing at \( x = 0 \); thus \( \Omega_1 = [-1, 0] \times [-1, 1] \) and \( \Omega_2 = [-1, 0] \times [-1, 1] \). We set the two boundary segments \( x = \pm 1 \) and \( \Gamma_N \) as the union of the segments \( y = \pm 1 \), as shown in Figure 1 (left). For the time interval \( [0, 1] \), we consider the following system
of two reaction-diffusion equations:

\[
\begin{align*}
    u_t - \Delta u &= f^u + \begin{cases} 
    u^2 - v(1 - v) & \text{in } \Omega_1 \\
    -v & \text{in } \Omega_2,
    \end{cases} \\
    v_t - \Delta v &= f^v + u & \text{in } \Omega_1 \cup \Omega_2,
\end{align*}
\]

(11)

with initial conditions \( u, v(0, \cdot) : \Omega \to \mathbb{R} \) and forcing terms \( f^{u,v} : [0, 1] \times \Omega \to \mathbb{R} \), fixed in order to yield as exact solution

\[
\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \cos t \\ \sin t \end{pmatrix} e^{(y^2 - 1)^2} \begin{cases} 
4x(1 + x) & \text{in } \Omega_1, \\
(-5x^3 + 4x + 1) & \text{in } \Omega_2.
\end{cases}
\]

(12)

The first component of the solution at \( t = 1 \) is shown in Figure 1 (right). Both components of the solution obey homogeneous Dirichlet and Neumann boundary conditions on \( \Gamma_D \) and \( \Gamma_N \), respectively. Further, it is compatible with the transmission conditions (5) with respect to the permeability \( p \equiv 4 \) for both components of the solution.

Numerical results are reported in Table 1 in the cases of linear and quadratic finite elements in space. The \( L^2(0,T;H^1) \) error rate (mean-square norm in time and mean square plus mean square derivative norm in space) of convergence are optimal, while the \( L^\infty(0,T;L^2(\Omega)) \) error rate (maximum norm in time with mean square norm in space) are, as expected, one-order suboptimal. The lost in convergence rate visible in the latest refinements is due to the time discretisation error.

As a second example, we present an application into the numerical simulation of molecular cellular signal transduction processes. Here the term transduction refers to the ensemble of the complex mechanisms put in place by nature in order to select the stimuli impinging on the cell. Indeed a typical transduction process comprises: the activation of internal signaling molecules which are set free to diffuse inside the cell, a cascade of reactions between the signaling molecules and other molecules inside the cell, and, if necessary, the translocation of the signaling molecules across a target cellular compartment,
\[ L^2(0,T; S) \quad L^\infty(0,T; L^2(\Omega)) \]

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Table 1: Example 1. Errors and convergence rates for linear (above) and quadratic (below) DG in space discretisations.

\( \ast \) the nucleus. Mathematically, we model the whole transduction mechanism in terms of a system of reaction-diffusion equations set on the relevant cellular compartments.

We consider in particular the simple model comprising two compartments: the cellular cytoplasm and the nucleus contained in it. This was introduced in \[5\] where the modelling details are thoroughly discussed. Homogeneous Neumann conditions apply to the cellular domain boundary while the purely diffusive interface condition \((5)\) with constant permeability is set on the interface boundary between the two compartments. The mode in \[5\] comprises of nine mixed hyperbolic/parabolic equations in total, is solved numerically using the IP-DG method described above.

Experimental evidence \[14\] shows that some molecular signaling molecules (\(e.g.\) tumour suppressors) take advantage of the cellular skeleton (the cytoplasmic microtubules) and a special set of proteins (the motor proteins) in order to get transported towards the nucleus in a directed fashion. This is taken into account by adding to the model a transport equation describing the dynamics of the signal-motor complex traveling towards the nucleus with constant speed. The hyperbolic, transport, equation is coupled to the parabolic, diffusion, system via the reaction terms modelling attachment and detachment to the microtubules.

Figure 2 shows the evolution of the concentration of an activated signalling species initially concentrated on a spot near the domain boundary. The transport mechanism ensures that the initial spot, instead of being diffused in all directions, is transported towards the nuclear compartment (the contour of which is visible through the jump in the concentration).
Figure 2: Numerical simulation of molecular signaling inside a biological cell

5 CONCLUSIONS

We proposed a new Interior Penalty Discontinuous Galerkin (IP-DG) finite element method for the solution of nonlinear convection-reaction-diffusion systems on partitioned subdomains arising in the modelling of mass transfer through semi-permeable membranes. Non-linear interface conditions are imposed at the sub-domain interfaces. A number of issues relating to the accuracy and numerical stability of the method have been addressed by this research. The problem considered is relevant to the modelling of chemical species passing through thin biological membranes and an example of the application of the
proposed method in the modelling of cellular signal transduction is given. A rigorous error analysis of the proposed method will be given elsewhere.

REFERENCES


