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**Space-time discontinuous Galerkin method  
for parabolic problems  
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# Space-Time Discontinuous Galerkin Method for Parabolic Problems in Time-Dependent Domains

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## Abstract

In this report a space-time discontinuous Galerkin (DG) finite element method for the solution of the advection-diffusion-reaction equation in time-dependent domains is presented and analyzed. The variational formulation is based on a combination of the space-time DG method developed by van der Vegt and van der Ven for hyperbolic partial differential equations and the DG algorithm for elliptic equations by Arnold, Brezzi, Cockburn and Marini.

Keywords: discontinuous Galerkin, parabolic problems, time-dependent domain.  
Mathematics Subject Classification: 65M60, 76M10, 35K20

## 1 Introduction

Fluid flow problems in time-dependent domains are observed in many engineering applications, for example in micro electromechanical systems. Performing experiments in this field is challenging and expensive, and analytical approaches are limited to simplified model. Numerical simulations provide an alternative technique to analyze fluid flow problems in complex time-dependent geometries within a reasonable computing time and accuracy. Discontinuous Galerkin (DG) finite element which provide great flexibility to discretize complex geometries in time-dependent flow domains, usually satisfy these requirements.

In this report we develop a space-time discontinuous Galerkin (DG) finite element method for linear advection-diffusion-reaction equations. We extend the space-time DG formulation in [16, 17] to include second-order partial differential equations. The space-time DG method has as key feature that time is treated as an extra dimension which makes the method particularly useful for problems with time-dependent flow domains. In addition, we analyze important properties of the new technique in the finite element framework, such as existence and uniqueness of the numerical solution. In the first part of the paper we formulate the space-time DG method for parabolic equations. Following the standard technique for DG methods for second-order partial differential equations (see for instance [1, 3, 6, 7]), the equation is rewritten as a first-order system by introducing an auxiliary variable. As no interelement continuity is imposed on the polynomial basis functions in the DG method, the well-posedness of the discrete formulation is achieved by introducing numerical fluxes. For second-order elliptic partial differential equations, [1, 2] give a complete analysis of all numerical fluxes available in the literature. After a comprehensive study [15], we use the numerical flux proposed by

Bassi and Rebay in [3]. This numerical flux is described in more detail in [6]. In order to give a full description of the new technique, we prove that the space-time DG finite element discretization has a unique solution, by extending the analysis given in [9, 10, 11, 12] to the space-time domain.

The organization of this report is as follows. First, a model problem for time-dependent parabolic partial differential equations is introduced in Section 2, followed by a discussion of the geometry of the space-time domain and elements. Next, the definitions of the finite element spaces and the trace operators related to the problem are given. Section 3 starts with the transformation of the model problem to the space-time framework and the weak formulation for the space-time DG method is derived. In Section 4 we prove the existence of a unique solution obtained with the space-time DG method for the linear advection-diffusion-reaction equation. Concluding remarks are drawn in Section 5.

## 2 Preliminaries

### 2.1 Model problem

Let  $\Omega_t$  be an open, bounded, time-dependent domain in  $\mathbb{R}^d$ , where  $d$  is the number of space dimensions. The closure of  $\Omega_t$  is  $\bar{\Omega}_t$  and the boundary of  $\Omega_t$  is denoted by  $\partial\Omega_t$ . Denoting  $\bar{x} = (x_1, \dots, x_d)$  as the space variables, we consider the time-dependent advection-diffusion-reaction equation in the domain  $\Omega_t$ :

$$\frac{\partial u}{\partial t} + \sum_{i=1}^d b_i(\bar{x}) \frac{\partial u}{\partial x_i} - \sum_{i,j=1}^d \frac{\partial}{\partial x_j} \left( D_{ij}(\bar{x}) \frac{\partial u}{\partial x_i} \right) + c(\bar{x})u = f(t, \bar{x}), \quad t \in [t_0, T], \quad (2.1)$$

where  $f \in L^2(\Omega_t)$  and  $c \in L^\infty(\Omega_t)$ ,  $c \geq 0$  are real-valued functions,  $b = \{b_i\}_{i=1}^d$  a vector function whose entries are Lipschitz continuous real-valued functions on  $\bar{\Omega}_t$  and  $D = \{D_{ij}\}_{i,j=1}^d$  a symmetric positive definite matrix on  $\bar{\Omega}_t$  whose entries are bounded, piecewise continuous real-valued functions. We denote by  $\bar{n} = \{n_i\}_{i=1}^d$  the normal vector to  $\partial\Omega_t$ . Using the same argument as in [12], we define

$$\begin{aligned} \partial_0\Omega_t &= \{\bar{x} \in \partial\Omega_t : \bar{n}^T D \bar{n} > 0\}, \\ \partial_-\Omega_t &= \{\bar{x} \in \partial\Omega_t \setminus \partial_0\Omega_t : b \cdot \bar{n} < 0\}, \quad \partial_+\Omega_t = \{\bar{x} \in \partial\Omega_t \setminus \partial_0\Omega_t : b \cdot \bar{n} \geq 0\}. \end{aligned}$$

We assign the sets  $\partial_-\Omega_t$  and  $\partial_+\Omega_t$  as the inflow and outflow boundary, respectively. Clearly,  $\partial\Omega_t = \partial_0\Omega_t \cup \partial_-\Omega_t \cup \partial_+\Omega_t$ . If  $\partial_0\Omega_t$  is nonempty, we further divide it into disjoint subsets  $\partial_D\Omega_t$  and  $\partial_M\Omega_t$  whose union is  $\partial_0\Omega_t$ , with  $\partial_D\Omega_t$  having a non-zero measure. The disjoint sets  $\partial_D\Omega_t$  and  $\partial_M\Omega_t$  are related to the Dirichlet and mixed or Robin boundary conditions, respectively. We supplement (2.1) with the initial condition

$$u = u_0 \quad \text{at } t = t_0, \quad (2.2)$$

with  $u_0$  a real-valued function on  $\Omega(t_0)$  and the boundary conditions:

$$u = g_D \quad \text{on } \partial_D\Omega_t, \quad \alpha u + \sum_{i,j=1}^d n_j D_{ij} \frac{\partial u}{\partial x_i} = g_M \quad \text{on } \partial_M\Omega_t, \quad (2.3)$$

where  $g_D, g_N$  are given functions on  $\partial_D\Omega_t$  and on  $\partial_M\Omega_t$ , respectively, and  $\alpha \geq 0$  a continuous function on  $\partial_M\Omega_t$ . We adopt the (physically reasonable) hypothesis [12] that  $b \cdot \bar{n} \geq 0$  on  $\partial_M\Omega_t$  whenever  $\partial_M\Omega_t$  is nonempty.

## 2.2 Geometry of space-time domain and elements

In the space-time discontinuous Galerkin discretization we do not make a distinction between space and time variables and directly consider a domain in  $\mathbb{R}^{d+1}$ . Let  $\mathcal{E} \subset \mathbb{R}^{d+1}$  be an open domain. A point  $x \in \mathbb{R}^{d+1}$  has coordinates  $(x_0, \bar{x}) = (x_0, x_1, \dots, x_d)$ , with  $t = x_0$  representing time. The space domain  $\Omega_t$  is redefined as the space-time domain  $\Omega_t := \{\bar{x} \in \mathbb{R}^d \mid (t, \bar{x}) \in \mathcal{E}\}$  for  $t \in [t_0, T]$ , where  $t_0$  and  $T$  represent the initial and final time of the evolution of the domain. The space-time domain boundary  $\partial\mathcal{E}$  consists of the hypersurfaces  $\Omega_{t_0} := \{x \in \partial\mathcal{E} \mid x_0 = t_0\}$ ,  $\Omega_T := \{x \in \partial\mathcal{E} \mid x_0 = T\}$ , and  $\mathcal{Q} := \{x \in \partial\mathcal{E} \mid t_0 < x_0 < T\}$ .

Next, we consider the time interval  $\mathcal{I} = (t_0, T)$ , partitioned by an ordered series of time levels  $t_0 < t_1 < \dots < t_{N_t} = T$ . Denoting the  $n$ th time interval as  $I_n = (t_n, t_{n+1})$ , we have  $\mathcal{I} = \cup_{n=0}^{N_t-1} I_n$ . The length of each time interval is defined as  $\Delta_n t = t_{n+1} - t_n$ . The space-time domain  $\mathcal{E}$  is then divided into  $N_t$  space-time slabs  $\mathcal{E}^n = \mathcal{E} \cap I_n$ . Each space-time slab  $\mathcal{E}^n$  is bounded by  $\Omega_{t_n}$ ,  $\Omega_{t_{n+1}}$ , and  $\mathcal{Q}^n = \partial\mathcal{E}^n \setminus (\Omega_{t_n} \cup \Omega_{t_{n+1}})$ .

We describe now the construction of the space-time elements  $K_j^n$  in  $\mathcal{E}^n$ . Let  $\Omega_{h,t_n}$  be an approximation to  $\Omega_{t_n}$  at time level  $t_n$ , with  $\Omega_{h,t_n} \rightarrow \Omega_{t_n}$  as  $h \rightarrow 0$ . Similarly,  $\Omega_{h,t_{n+1}}$  is an approximation to  $\Omega_{t_{n+1}}$  at time level  $t_{n+1}$ . The domain  $\Omega_{h,t_n}$  is divided into  $N_n$  non-overlapping spatial elements  $K_j^n = K_j(t_n)$ . At time level  $t_{n+1}$  the spatial elements  $K_j^{n+1} = K_j(t_{n+1})$  are obtained by mapping  $K_j^n$  to their new position at  $t = t_{n+1}$ . Each element  $K_j^n$  is now obtained by connecting elements  $K_j^n$  and  $K_j^{n+1}$  using linear interpolation in time. The element boundary  $\partial K_j^n$  is denoted as the union of open faces of  $K_j^n$ , which contains three parts  $K_j(t_n^+) = \lim_{\epsilon \downarrow 0} K_j(t_n + \epsilon)$ ,  $K_j(t_{n+1}^-) = \lim_{\epsilon \downarrow 0} K_j(t_{n+1} - \epsilon)$ , and  $\mathcal{Q}_j^n = \partial K_j^n \setminus (K_j(t_n^+) \cup K_j(t_{n+1}^-))$ . The definitions are completed with the tessellation  $\mathcal{T}_h^n$ , which consists of all space-time elements in the space-time slab  $\mathcal{E}_h^n$ , an approximation to  $\mathcal{E}^n$ , and  $\mathcal{T}_h = \cup_{n=0}^{N_t-1} \mathcal{T}_h^n$ , the union of all space-time elements in the space-time domain  $\mathcal{E}_h$ , which is an approximation to  $\mathcal{E}$ .

All the faces  $S$  in the space-time discretization are grouped into the set  $\mathcal{F}$ , which is the union of two disjoint sets: the set  $\mathcal{F}_{\text{int}}$ , which consists of all faces in  $\mathcal{E}_h$  shared by two elements, and the set  $\mathcal{F}_{\text{bnd}}$ , which consists of all faces at the boundary of  $\mathcal{E}_h$ . We also consider the faces in the space-time slab  $\mathcal{E}_h^n$ . We denote by  $\mathcal{S}^n$  the set of open faces in  $\mathcal{E}_h^n$ . First, we define the set  $\mathcal{S}_I^n \subset \mathcal{S}^n$ . Each face  $S \in \mathcal{S}_I^n$  is connected to two space-time elements within the same slab. At the space-time slab boundary  $\mathcal{Q}^n$ , we define two sets of boundary faces; the set  $\mathcal{S}_D^n$  with a Dirichlet boundary condition and the set  $\mathcal{S}_M^n$  with a mixed boundary condition. The sets  $\mathcal{S}_I^n$  and  $\mathcal{S}_D^n$  are grouped into the set  $\mathcal{S}_{ID}^n$ .

## 2.3 Function spaces and trace operators

In this section, we introduce the standard definitions of the Sobolev spaces for real-valued functions in the domains  $\Omega_t$  and  $\mathcal{E}$ , taken from [13]. Although the definition of the Sobolev space in [13] is for a fixed space domain, by changing of variables, the definition also holds for a time-dependent domain  $\Omega_t$ .

First, in the domain  $\Omega_t$  we introduce the standard definition of the Sobolev space  $H^s(\Omega_t)$  for real-valued functions, with  $s \in \mathbb{R}$ . We refer to [4] for more details. When  $s = 0$ , the space  $H^0(\Omega_t)$  is denoted as  $L^2(\Omega_t)$ , equipped with standard inner-product and norm

$$(w, v)_{L^2(\Omega_t)} := \int_{\Omega_t} w v d\mathcal{K}, \quad \|v\|_{L^2(\Omega_t)} := (v, v)_{L^2(\Omega_t)}^{1/2}, \quad (2.4)$$

and for nonnegative integer  $m$ , the Sobolev norm and semi-norm are defined as

$$\|v\|_{H^m(\Omega_t)} := \left( \sum_{|\gamma| \leq m} \|D^\gamma v\|_{L^2(\Omega_t)}^2 \right)^{\frac{1}{2}}, \quad |u|_{H^m(\Omega_t)} := \left( \sum_{|\gamma|=m} \|D^\gamma v\|_{L^2(\Omega_t)}^2 \right)^{\frac{1}{2}}, \quad (2.5)$$

where  $D^\gamma = (\partial/\partial x_1)^{\gamma_1} \dots (\partial/\partial x_d)^{\gamma_d}$  denotes the usual partial derivative with multi-index  $\gamma = (\gamma_1, \dots, \gamma_d)$ ,  $\gamma_i$  non-negative integers, and the length of  $\gamma$  given by  $|\gamma| := \sum_{i=1}^d \gamma_i$ .

The standard definition of the Sobolev space  $H^s(\mathcal{E})$ , with  $s \in \mathbb{R}$ , is similar as the definition of the Sobolev space in  $\Omega_t$ , except with the extension of one dimension. For  $s = 1$ , we also introduce the space  $H^{1,0}(\mathcal{E}) = L^2((t_0, T); H^1(\Omega_t))$  which is the space consisting of the elements of the space  $L^2(\mathcal{E})$  having partial derivatives  $\partial/\partial x_i$ ,  $i = 1, \dots, d$ , square summable on  $\mathcal{E}$ .

Now we introduce the finite element space associated with the tessellation  $\mathcal{T}_h$ . For simplicity of notation, in the remaining part of this section we denote the space-time element with  $\mathcal{K}$ . We assume that each element  $\mathcal{K}$  is an image of a fixed master element  $\hat{\mathcal{K}}$ , i.e.  $\mathcal{K} = G_{\mathcal{K}}(\hat{\mathcal{K}})$  for all  $\mathcal{K} \in \mathcal{T}_h$ , where  $\hat{\mathcal{K}}$  is the open unit hypercube in  $\mathbb{R}^{d+1}$ . Analogously, for  $k \geq 1$ ,  $\mathcal{Q}_k(\hat{\mathcal{K}})$  is defined as the set of all tensor-product polynomials on  $\hat{\mathcal{K}}$  of degree  $k$  in each coordinate direction.

To each element  $\mathcal{K}$  we assign a nonnegative integer  $p_{\mathcal{K}}$  (local polynomial degree) and a nonnegative integer  $s_{\mathcal{K}}$  (local Sobolev index), and collect  $p_{\mathcal{K}}$  and  $s_{\mathcal{K}}$  in the vectors:  $\mathbf{p} = \{p_{\mathcal{K}} : \mathcal{K} \in \mathcal{T}_h\}$  and  $\mathbf{s} = \{s_{\mathcal{K}} : \mathcal{K} \in \mathcal{T}_h\}$ . We consider the finite element space

$$V_h := \{u \in L^2(\mathcal{E}_h) : u|_{\mathcal{K}} \circ G_{\mathcal{K}} \in \mathcal{Q}_{p_{\mathcal{K}}}(\hat{\mathcal{K}}), \forall \mathcal{K} \in \mathcal{T}_h\}. \quad (2.6)$$

Further, we assign to  $\mathcal{T}_h$  the broken Sobolev space  $H^s(\mathcal{E}_h, \mathcal{T}_h) := \{u \in L^2(\mathcal{E}_h) : u|_{\mathcal{K}} \in H^{s_{\mathcal{K}}}(\mathcal{K}), \forall \mathcal{K} \in \mathcal{T}_h\}$ , equipped with the broken Sobolev norm and corresponding semi-norm, respectively,

$$\|u\|_{\mathbf{s}, \mathcal{T}_h} := \left( \sum_{\mathcal{K} \in \mathcal{T}_h} \|u\|_{H^{s_{\mathcal{K}}}(\mathcal{K})}^2 \right)^{\frac{1}{2}}, \quad |u|_{\mathbf{s}, \mathcal{T}_h} := \left( \sum_{\mathcal{K} \in \mathcal{T}_h} |u|_{H^{s_{\mathcal{K}}}(\mathcal{K})}^2 \right)^{\frac{1}{2}}. \quad (2.7)$$

For  $u \in H^1(\mathcal{E}_h, \mathcal{T}_h)$ , we define the broken gradient  $\nabla_h u$  of  $u$  by  $(\nabla_h u)|_{\mathcal{K}} := \nabla(u|_{\mathcal{K}}), \forall \mathcal{K} \in \mathcal{T}_h$ . In the derivation and analysis of the numerical discretization we will also make use of the auxiliary space  $\Sigma_h$ :

$$\Sigma_h = \{\tau \in L^2(\mathcal{E}_h)^{d+1} : \tau|_{\mathcal{K}} \circ G_{\mathcal{K}} \in \mathcal{Q}_{p_{\mathcal{K}}}(\hat{\mathcal{K}})^{d+1}, \forall \mathcal{K} \in \mathcal{T}_h\}.$$

For consistency reasons, we require  $\nabla_h V_h \subset \Sigma_h$ . The trace of functions  $v \in V_h$  at the boundary  $\partial\mathcal{K}$  is defined as:

$$v_{\mathcal{K}}^{\pm} = \lim_{\epsilon \downarrow 0} v(x \pm \epsilon n_{\mathcal{K}}),$$

with  $n_{\mathcal{K}}$  the unit outward space-time normal vector at  $\partial\mathcal{K}$ . The trace of functions  $\tau \in \Sigma_h$  is defined similarly.

Next, we define the *average*  $\{\!\{ \cdot \}\!\}$  and *jump*  $[\![ \cdot ]\!]$  operators as trace operators for the sets  $\mathcal{F}_{\text{int}}$  and  $\mathcal{F}_{\text{bnd}}$ . Note that functions  $v \in V_h$  and  $\tau \in \Sigma_h$  are multivalued at internal faces  $S \in \mathcal{F}_{\text{int}}$ . Introducing the functions  $v_i := v|_{\mathcal{K}_i}$ ,  $\tau_i := \tau|_{\mathcal{K}_i}$ ,  $n_i := n|_{\mathcal{K}_i}$ , the average operator is defined as:

$$\{\!\{ v \}\!\} = (v_i^- + v_j^-)/2, \quad \text{on } S \in \mathcal{F}_{\text{int}}, \quad \{\!\{ v \}\!\} = v^-, \quad \text{on } S \in \mathcal{F}_{\text{bnd}}, \quad (2.8a)$$

$$\llbracket \tau \rrbracket = (\tau_i^- + \tau_j^-)/2, \quad \text{on } S \in \mathcal{F}_{\text{int}}, \quad \llbracket \tau \rrbracket = \tau^-, \quad \text{on } S \in \mathcal{F}_{\text{bnd}}, \quad (2.8b)$$

while the jump operator is defined as:

$$[[v]] = v_i^- n_i + v_j^- n_j, \quad \text{on } S \in \mathcal{F}_{\text{int}}, \quad [[v]] = v^- n, \quad \text{on } S \in \mathcal{F}_{\text{bnd}}, \quad (2.8c)$$

$$[[\tau]] = \tau_i^- \cdot n_i + \tau_j^- \cdot n_j, \quad \text{on } S \in \mathcal{F}_{\text{int}}, \quad [[\tau]] = \tau^- \cdot n, \quad \text{on } S \in \mathcal{F}_{\text{bnd}}, \quad (2.8d)$$

with  $i$  and  $j$  the indices of the two elements  $\mathcal{K}_i$  and  $\mathcal{K}_j$  which connect to the face  $S$ . The unit normal vectors  $n|_{\mathcal{K}_i}$  and  $n|_{\mathcal{K}_j}$  are defined pointing exterior to  $\mathcal{K}_i$  and  $\mathcal{K}_j$ , respectively. Note that the jump  $[[v]]$  is a vector parallel to the normal and the jump  $[[\tau]]$  is a scalar quantity. We will also need the spatial jump operator  $\langle\langle \cdot \rangle\rangle$  for functions  $v \in V_h$ , which is defined as:

$$\langle\langle v \rangle\rangle = v_i^- \bar{n}_i + v_j^- \bar{n}_j, \quad \text{on } S \in \mathcal{F}_{\text{int}}, \quad \langle\langle v \rangle\rangle = v^- \bar{n}, \quad \text{on } S \in \mathcal{F}_{\text{bnd}}. \quad (2.9)$$

## 2.4 Lifting operators

The derivation of the primal space-time DG formulation requires several trace lifting operators. First, we define a linear global lifting operator  $R_{g_D} : (L^2(\mathcal{F}))^{d+1} \rightarrow \Sigma_h$  for every  $q, \phi \in \Sigma_h$  as:

$$\sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} R_{g_D}(\phi) \cdot q d\mathcal{K} = - \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} \int_S \phi \cdot \{\{q\}\} dS + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_D^n} \int_S g_D n \cdot q dS. \quad (2.10a)$$

We also define the linear global lifting operator  $R : (L^2(\mathcal{F}))^{d+1} \rightarrow \Sigma_h$  as

$$\sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} R(\phi) \cdot q d\mathcal{K} = - \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} \int_S \phi \cdot \{\{q\}\} dS, \quad (2.10b)$$

and we notice the following relationship between these operators:

$$\sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} R_{g_D}(\phi) \cdot q d\mathcal{K} = \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} R(\phi) \cdot q d\mathcal{K} + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_D^n} \int_S g_D n \cdot q dS. \quad (2.10c)$$

Note that lifting operators  $R, R_{g_D}$  are equal to zero on  $S \in \mathcal{S}_M^n$ . For each face  $S \in \mathcal{S}_{ID}^n$  we also define local lifting operators  $r_S, r_{S,g_D} : (L^2(S))^{d+1} \rightarrow \Sigma_h$  as

$$\sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} r_S(\phi) \cdot q d\mathcal{K} = - \int_S \phi \cdot \{\{q\}\} dS, \quad \forall q, \phi \in \Sigma_h, \quad \text{on } S \in \mathcal{S}_{ID}^n, \quad (2.11a)$$

and

$$\sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} r_{S,g_D}(\phi) \cdot q d\mathcal{K} = \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} r_S(\phi) \cdot q d\mathcal{K} + \int_S g_D n \cdot q dS, \quad \forall q, \phi \in \Sigma_h, \quad \text{on } S \in \mathcal{S}_D^n. \quad (2.11b)$$

The support of the operators  $r_S, r_{S,g_D}$  is contained inside the element(s) that share the face  $S$ . The following relationship between  $R$  and  $r_S$  holds [14]:

$$R = \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} r_S, \quad \text{on } \mathcal{E}_h. \quad (2.12)$$

We will also use the spatial part of the lifting operators  $R, r_S$ , denoted by  $\bar{R}$  and  $\bar{r}_S$ , which is obtained by setting the first component of  $R$  and  $r_S$  equal to zero.

### 3 Space-Time DG Discretization

#### 3.1 Space-time formulation of parabolic equations

In this section we will reformulate problem (2.1)-(2.3) in the space-time framework. We introduce the vector function  $B \in \mathbb{R}^{d+1}$  and the symmetric matrix  $A \in \mathbb{R}^{(d+1) \times (d+1)}$  as:

$$B = \begin{pmatrix} 1 \\ b \end{pmatrix}, \quad A = \begin{pmatrix} 0 & 0 \\ 0 & D \end{pmatrix},$$

with  $D$  the symmetric positive definite matrix defined in Section 2.1, which admits a unique square root  $D^{1/2}$ .

The parabolic partial differential equation (2.1) can now be transformed into a space-time formulation as:

$$-\nabla \cdot (A\nabla u - Bu) + cu = f, \quad \text{in } \mathcal{E}, \quad (3.1)$$

where  $\nabla = (\frac{\partial}{\partial x_0}, \frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_d})^T$  denotes the gradient operator in  $\mathbb{R}^{d+1}$ . Later we will also use the notation  $\bar{\nabla}$  to denote the spatial gradient operator in  $\mathbb{R}^d$ , defined as  $\bar{\nabla} = (\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_d})^T$ . The unit outward normal vector at  $\partial\mathcal{E}$  is denoted with  $n$ . The domain boundary  $\partial\mathcal{E}$  is divided into disjoint subsets  $\partial\mathcal{E} = \Gamma_0 \cup \Gamma_- \cup \Gamma_+$ , where:

$$\Gamma_0 = \{x \in \partial\mathcal{E} : n^T A n > 0\}, \quad \Gamma_- = \{x \in \partial\mathcal{E} \setminus \Gamma_0 : B \cdot n < 0\}, \quad \Gamma_+ = \{x \in \partial\mathcal{E} \setminus \Gamma_0 : B \cdot n \geq 0\}.$$

Further, we divide  $\Gamma_0$  into disjoint subsets  $\Gamma_D$  and  $\Gamma_M$ , with  $\Gamma_D$  nonempty and relatively open in  $\partial\mathcal{E}$ . The initial and boundary conditions in the space-time formulation are written as

$$u = u_0 \quad \text{on } \Gamma_-, \quad u = g_D \quad \text{on } \Gamma_D, \quad \alpha u + n \cdot (A\nabla u) = g_M \quad \text{on } \Gamma_M. \quad (3.2)$$

The parabolic partial differential equation (3.1) with initial and boundary conditions (3.2) has a unique solution  $u \in H^{1,0}(\mathcal{E})$  [13]. Introducing an auxiliary variable  $\sigma = A\nabla u$ , we can rewrite (3.1) as a first-order system:

$$-\nabla \cdot (\sigma - Bu) + cu = f, \quad (3.3a)$$

$$\sigma = A\nabla u. \quad (3.3b)$$

In the next section we will discuss in detail the derivation of the weak formulation of (3.3) in the space-time framework.

#### 3.2 Formulation of the auxiliary variable

First, we consider the equation for the auxiliary variable  $\sigma$  (3.3b). Multiplying (3.3b) with an arbitrary test function  $\tau \in \Sigma_h$  and integrating over element  $\mathcal{K} \in \mathcal{T}_h$ , we obtain:

$$\int_{\mathcal{K}} \sigma \cdot \tau d\mathcal{K} = \int_{\mathcal{K}} A\nabla u \cdot \tau d\mathcal{K}, \quad \forall \tau \in \Sigma_h. \quad (3.4)$$

Next, we substitute  $\sigma$  and  $u$  with  $\sigma_h \in \Sigma_h$  and  $u_h \in V_h$ , and after integration by parts twice, we obtain:

$$\sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} \sigma_h \cdot \tau d\mathcal{K} = \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} A\nabla_h u_h \cdot \tau d\mathcal{K} + \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial\mathcal{K}} A(\hat{u}_h - u_h^-) n \cdot \tau^- d\mathcal{K}, \quad \forall \tau \in \Sigma_h. \quad (3.5)$$

The variable  $\hat{u}_h$  is the *numerical flux* that must be defined to account for the multivalued trace at  $\partial\mathcal{K}$ . By choosing  $\hat{u}_h = u_h$  at the element boundaries  $K_j(t_{n+1}^-)$  and  $K_j(t_n^+)$ , we only have to consider the weak formulation in a space-time slab  $\mathcal{E}_h^n$  and (3.5) can be written as

$$\sum_{\mathcal{K} \in \mathcal{T}_h^n} \int_{\mathcal{K}} \sigma_h \cdot \tau d\mathcal{K} = \sum_{\mathcal{K} \in \mathcal{T}_h^n} \int_{\mathcal{K}} A \nabla_h u_h \cdot \tau d\mathcal{K} + \sum_{\mathcal{K} \in \mathcal{T}_h^n} \int_{\mathcal{Q}_j^n} A(\hat{u}_h - u_h^-) n \cdot \tau^- d\partial\mathcal{K}, \quad \forall \tau \in \Sigma_h. \quad (3.6)$$

For the numerical flux  $\hat{u}_h$  at the faces  $\mathcal{Q}_j^n$ , we make the same choice as in [3, 6]

$$\hat{u}_h = \llbracket u_h \rrbracket, \quad \text{on } \mathcal{S}_I^n, \quad \hat{u}_h = g_D, \quad \text{on } \mathcal{S}_D^n, \quad \hat{u}_h = u_h^-, \quad \text{on } \mathcal{S}_M^n.$$

Replacing  $\hat{u}_h$  with these choices, and after summation of the integrals over the element boundaries  $\mathcal{Q}_j^n$  we obtain the following relation for the boundary integrals:

$$\sum_{\mathcal{K} \in \mathcal{T}_h^n} \int_{\mathcal{Q}_j^n} A(\hat{u}_h - u_h^-) n \cdot \tau^- d\partial\mathcal{K} = - \sum_{S \in \mathcal{S}_{ID}^n} \int_S \llbracket u_h \rrbracket \cdot \llbracket A\tau \rrbracket dS + \sum_{S \in \mathcal{S}_D^n} \int_S g_D n \cdot A\tau dS, \quad (3.7)$$

where we use the average and jump operators, the symmetry properties of matrix  $A$  and the fact that each interior face  $S \in \mathcal{S}_I^n$  occurs twice in the summation over all elements  $\mathcal{K} \in \mathcal{T}_h$ . This relation is similar to the formulation derived in [5], see also [6] for more details. If we introduce the lifting operator (2.10a) and sum over all space-time slabs, we can write (3.7) as

$$\sum_{n=0}^{N_t-1} \left( - \sum_{S \in \mathcal{S}_{ID}^n} \int_S \llbracket u_h \rrbracket \cdot \llbracket A\tau \rrbracket dS + \sum_{S \in \mathcal{S}_D^n} \int_S g_D n \cdot A\tau dS \right) = \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} R_{g_D}(\llbracket u_h \rrbracket) \cdot A\tau d\mathcal{K}, \quad (3.8)$$

where we replace  $\phi$  and  $q$  in (2.10a) with  $\llbracket u_h \rrbracket$  and  $A\tau$ , respectively. Using the relation (3.8), the symmetry properties of matrix  $A$  and after summation over all space-time slabs, we can write (3.6) as

$$\sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} \sigma_h \cdot \tau d\mathcal{K} = \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} A \nabla_h u_h \cdot \tau d\mathcal{K} + \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} A R_{g_D}(\llbracket u_h \rrbracket) \cdot \tau d\mathcal{K}, \quad \forall \tau \in \Sigma_h, \quad (3.9)$$

and we can express  $\sigma_h \in \Sigma_h$  as:

$$\sigma_h = A \nabla_h u_h + A R_{g_D}(\llbracket u_h \rrbracket), \quad \text{a.e. } x \in \mathcal{E}_h. \quad (3.10)$$

### 3.3 Weak formulation of space-time DG method

The weak formulation for (3.3a) is obtained if we multiply (3.3a) with arbitrary test functions  $v \in V_h$ , integrate by parts over element  $\mathcal{K}$ , and substitute  $u, \sigma$  with  $u_h \in V_h, \sigma_h \in \Sigma_h$ , respectively, such that for all  $v \in V_h$  we obtain:

$$\sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} ((\sigma_h - B u_h) \cdot \nabla_h v + c u_h v) d\mathcal{K} - \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial\mathcal{K}} (\hat{\sigma}_h - B \hat{u}_h) \cdot n v^- d\partial\mathcal{K} = \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} f v d\mathcal{K}, \quad (3.11)$$

where we replace  $u_h, \sigma_h$  at  $\partial\mathcal{K}$  with the numerical fluxes  $\hat{u}_h, \hat{\sigma}_h$ , to account for the multivalued traces at  $\partial\mathcal{K}$ .



The summation over the boundaries of the space-time elements in (3.11) involving the variable  $\hat{\sigma}_h$  is of the form

$$\sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial \mathcal{K}} \hat{\sigma}_h \cdot n v^- d\partial \mathcal{K}$$

and can also be written as a sum on all faces  $S \in \mathcal{F}$ . For each internal face  $S \in \mathcal{F}_{\text{int}}$ , shared by elements  $\mathcal{K}_i$  and  $\mathcal{K}_j$ , there are two contributions from the integrals over the element boundaries:

$$\int_S \hat{\sigma}_h \cdot n_i v_i^- dS + \int_S \hat{\sigma}_h \cdot n_j v_j^- dS = \int_S \hat{\sigma}_h \cdot \llbracket v \rrbracket dS, \quad (3.12)$$

with  $v_l := v|_{\mathcal{K}_l}$  and  $n_l := n|_{\mathcal{K}_l}$ ,  $l = i, j$ . Here we use the jump operator defined in (2.8c). For a boundary face  $S \in \mathcal{F}_{\text{bnd}}$ , we obtain, using the same jump operator

$$\int_S \hat{\sigma}_h \cdot n_j v_j^- dS = \int_S \hat{\sigma}_h \cdot \llbracket v \rrbracket dS. \quad (3.13)$$

If we introduce (3.12)-(3.13) into the weak formulation (3.11), we obtain

$$\begin{aligned} \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} ((\sigma_h - B u_h) \cdot \nabla_h v + c u_h v) d\mathcal{K} - \sum_{S \in \mathcal{F}} \int_S \hat{\sigma}_h \cdot \llbracket v \rrbracket dS \\ + \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial \mathcal{K}} B \hat{u}_h \cdot n v^- d\partial \mathcal{K} = \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} f v d\mathcal{K}, \quad \forall v \in V_h. \end{aligned} \quad (3.14)$$

Note that we only replace the summation over the element boundaries with a summation over the faces for the integrals with variable  $\hat{\sigma}_h$ . We will discuss the summation over the element boundary for the integrals with variable  $\hat{u}_h$  later in this report.

The next step is to find appropriate choices for the numerical fluxes. We separate the numerical fluxes into an *advective flux*  $B \hat{u}_h$  and a *diffusive flux*  $\hat{\sigma}_h$ . To ensure continuity and causality of the flux, we replace  $B \hat{u}_h$  with a monotone upwind flux  $H(u_h^-, u_h^+, B)$ , which is consistent and conservative, while  $\hat{\sigma}_h$  is replaced with  $\{\{\sigma_h\}\}$ , the average operator defined in (2.8b). After this replacement, the weak formulation (3.14) can be written as

$$\begin{aligned} \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} ((\sigma_h - B u_h) \cdot \nabla_h v + c u_h v) d\mathcal{K} - \sum_{S \in \mathcal{F}} \int_S \{\{\sigma_h\}\} \cdot \llbracket v \rrbracket dS \\ + \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial \mathcal{K}} H(u_h^-, u_h^+, B) \cdot n v^- d\partial \mathcal{K} = \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} f v d\mathcal{K}, \quad \forall v \in V_h. \end{aligned} \quad (3.15)$$

Using (3.10), we can eliminate  $\sigma_h$  from the weak formulation and obtain the primal formulation for  $u_h$ :

$$\begin{aligned} \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} \left( (A \nabla_h u_h + A R_{g_D}(\llbracket u_h \rrbracket) - B u_h) \cdot \nabla_h v + c u_h v \right) d\mathcal{K} \\ - \sum_{S \in \mathcal{F}} \int_S (A \{\{\nabla_h u_h\}\} + A \{\{R_{g_D}(\llbracket u_h \rrbracket)\}\}) \cdot \llbracket v \rrbracket dS \\ + \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial \mathcal{K}} H(u_h^-, u_h^+, B) \cdot n v^- d\partial \mathcal{K} = \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} f v d\mathcal{K}, \quad \forall v \in V_h, \end{aligned} \quad (3.16)$$

since the average operator  $\{\!\!\{\cdot\}\!\!\}$  is linear. As the lifting operator  $R_{g_D}$  has nonzero values only on faces  $S \in \mathcal{S}_{ID}^n$ , we have the following relation

$$\begin{aligned} - \sum_{S \in \mathcal{F}} \int_S A\{\!\!\{R_{g_D}(\llbracket u_h \rrbracket)\}\!\!\} \cdot \llbracket v \rrbracket dS &= - \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} \int_S A\{\!\!\{R_{g_D}(\llbracket u_h \rrbracket)\}\!\!\} \cdot \llbracket v \rrbracket dS \\ &= \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} AR_{g_D}(\llbracket u_h \rrbracket) \cdot R(\llbracket v \rrbracket) d\mathcal{K}, \end{aligned} \quad (3.17)$$

using the lifting operator  $R$  (2.10b). Due to the symmetry properties of matrix  $A$  and using the lifting operator  $R_{g_D}$  (2.10a) we also have the relation

$$\begin{aligned} \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} AR_{g_D}(\llbracket u_h \rrbracket) \cdot \nabla_h v d\mathcal{K} &= - \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} \int_S \llbracket u_h \rrbracket \cdot A\{\!\!\{\nabla_h v\}\!\!\} dS \\ &\quad + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_D^n} \int_S g_D n \cdot A \nabla_h v dS. \end{aligned} \quad (3.18)$$

Following a similar approach as in [6], we replace the contribution from the global lifting operators  $R, R_{g_D}$  with the local lifting operators  $r_S, r_{S,g_D}$  defined in (2.11a)-(2.11b), using the relation

$$\sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} AR_{g_D}(\llbracket u_h \rrbracket) \cdot R(\llbracket v \rrbracket) d\mathcal{K} \cong \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} \eta_0 \int_{\mathcal{E}_h} Ar_{S,g_D}(\llbracket u_h \rrbracket) \cdot r_S(\llbracket v \rrbracket) d\mathcal{K}. \quad (3.19)$$

In Section 4 we will derive a sufficient value for the constant  $\eta_0 > 0$  to guarantee a stable and unique solution. The advantage of this replacement is that the stiffness matrix in the weak formulation (with the local lifting operators) is considerably sparser than the stiffness matrix resulting from the weak formulation with the global lifting operators. We refer to [2, 6] for further explanation about this remark.

The weak formulation for  $u_h \in V_h$  is then written as:

$$\begin{aligned} &\sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} \left( (A \nabla_h u_h - B u_h) \cdot \nabla_h v + c u_h v \right) d\mathcal{K} \\ &- \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} \int_S (\llbracket u_h \rrbracket \cdot A\{\!\!\{\nabla_h v\}\!\!\} + A\{\!\!\{\nabla_h u_h\}\!\!\} \cdot \llbracket v \rrbracket) dS + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_M^n} \int_S \alpha u_h^- v^- dS \\ &+ \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} \eta_0 \int_{\mathcal{E}_h} Ar_{S,g_D}(\llbracket u_h \rrbracket) \cdot r_S(\llbracket v \rrbracket) d\mathcal{K} + \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial \mathcal{K}} H(u_h^-, u_h^+, B) \cdot n v^- d\partial \mathcal{K} \\ &= \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} f v d\mathcal{K} - \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_D^n} \int_S g_D n \cdot A \nabla_h v^- dS + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_M^n} \int_S g_M v^- dS, \quad \forall v \in V_h, \end{aligned} \quad (3.20)$$

where we introduce the boundary condition  $A \nabla_h u_h \cdot n = g_M - \alpha u_h$  at  $S \in \mathcal{S}_M^n$ . Now we discuss the integrals over the element boundary for the numerical flux  $H(u_h^-, u_h^+, B)$ . As in

[10], each element boundary  $\partial\mathcal{K}$  can be decomposed into the union of four disjoint boundaries

$$\begin{aligned}\partial\mathcal{K} &\equiv \partial_+\mathcal{K} \cup (\partial_-\mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)) \cup (\partial_-\mathcal{K} \cap \Gamma_-) \cup (\partial_-\mathcal{K} \cap \Gamma_D) \\ &\equiv (\partial_+\mathcal{K} \cap \Gamma_+) \cup (\partial_+\mathcal{K} \setminus \Gamma_+) \cup (\partial_-\mathcal{K} \cap (\Gamma_- \cup \Gamma_D)) \cup (\partial_-\mathcal{K} \setminus (\Gamma_- \cup \Gamma_D))\end{aligned}\quad (3.21)$$

with

$$\partial_-\mathcal{K} := \{x \in \partial\mathcal{K} : B \cdot n_{\mathcal{K}} < 0\}, \quad \partial_+\mathcal{K} := \{x \in \partial\mathcal{K} : B \cdot n_{\mathcal{K}} \geq 0\}.$$

To ensure continuity and causality of the advective flux, we choose

$$\begin{aligned}H(u_h^-, u_h^+, B) &= B u_h^-, \text{ for } \partial_+\mathcal{K}, & H(u_h^-, u_h^+, B) &= B u_h^+, \text{ for } \partial_-\mathcal{K} \setminus (\Gamma_- \cup \Gamma_D), \\ H(u_h^-, u_h^+, B) &= B u_0, \text{ for } \partial_-\mathcal{K} \cap \Gamma_-, & H(u_h^-, u_h^+, B) &= B g_D, \text{ for } \partial_-\mathcal{K} \cap \Gamma_D,\end{aligned}$$

such that for each element  $\mathcal{K}$  we have the following relation

$$\begin{aligned}\int_{\partial\mathcal{K}} H(u_h^-, u_h^+, B) \cdot n v^- d\partial\mathcal{K} &= \int_{\partial_+\mathcal{K}} B u_h^- \cdot n v^- d\partial\mathcal{K} + \int_{\partial_-\mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)} B u_h^+ \cdot n v^- d\partial\mathcal{K} \\ &\quad + \int_{\partial_-\mathcal{K} \cap \Gamma_-} B u_0 \cdot n v^- d\partial\mathcal{K} + \int_{\partial_-\mathcal{K} \cap \Gamma_D} B g_D \cdot n v^- d\partial\mathcal{K}.\end{aligned}\quad (3.22)$$

Introducing the bilinear forms  $a : V_h \times V_h \rightarrow \mathbb{R}$ ,  $a_a : V_h \times V_h \rightarrow \mathbb{R}$ ,  $a_d : V_h \times V_h \rightarrow \mathbb{R}$  as

$$a(u_h, v) = a_a(u_h, v) + a_d(u_h, v), \quad (3.23)$$

defined by

$$\begin{aligned}a_a(u_h, v) &= \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} (-B u_h \cdot \nabla_h v + c u_h v) d\mathcal{K} + \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial_+\mathcal{K}} B \cdot n u_h^- v^- d\partial\mathcal{K} \\ &\quad + \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial_-\mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)} B \cdot n u_h^+ v^- d\partial\mathcal{K},\end{aligned}\quad (3.24a)$$

$$\begin{aligned}a_d(u_h, v) &= \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} D \bar{\nabla}_h u_h \cdot \bar{\nabla}_h v d\mathcal{K} \\ &\quad - \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{TD}^n} \int_S (\langle\langle u_h \rangle\rangle \cdot D \{\{\bar{\nabla}_h v\}\} + D \{\{\bar{\nabla}_h u_h\}\} \cdot \langle\langle v \rangle\rangle) dS \\ &\quad + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_M^n} \int_S \alpha u_h^- v^- dS + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{TD}^n} \eta_0 \int_{\mathcal{E}_h} D \bar{r}_S(\llbracket u_h \rrbracket) \cdot \bar{r}_S(\llbracket v \rrbracket) d\mathcal{K},\end{aligned}\quad (3.24b)$$

and the functional  $\ell : V_h \rightarrow \mathbb{R}$ , defined by

$$\begin{aligned}\ell(v) &= \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} f v d\mathcal{K} - \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_D^n} \int_S g_D \bar{n} \cdot D \bar{\nabla}_h v^- dS + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_M^n} \int_S g_M v^- dS \\ &\quad - \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_D^n} \eta_0 \int_S g_D D \bar{n} \cdot \bar{r}_S(\llbracket v \rrbracket) dS - \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial_-\mathcal{K} \cap \Gamma_-} B \cdot n u_0 v^- d\partial\mathcal{K} \\ &\quad - \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial_-\mathcal{K} \cap \Gamma_D} B \cdot n g_D v^- d\partial\mathcal{K},\end{aligned}\quad (3.24c)$$

we obtain the space-time DG method for advection-diffusion-reaction equation (2.1):

Find a  $u_h \in V_h$  such that:

$$a(u_h, v) = \ell(v) \quad \forall v \in V_h. \quad (3.25)$$

In the bilinear forms  $a_d$  and  $a_a$  and the functional  $\ell$ , we use the spatial gradient operator  $\bar{\nabla}$ , the spatial jump operator  $\llbracket \cdot \rrbracket$  and spatial lifting operator  $\bar{r}_S$  defined earlier in this report.

## 4 Analysis of the Existence of a Unique DG Solution

In this section we prove the existence of a unique solution of (3.25). First we show that the bilinear form (3.23) is coercive. Here we extend the proof described in [9, 10, 11, 12] to the space-time formulation. As we use similar lifting operators  $R$  and  $r_S$  as in [6], the proof involving these terms follows the same lines as used in [6].

First, we define the positive function  $c_0$  by

$$(c_0(x))^2 = c(x) + \frac{1}{2} \nabla \cdot B(x), \quad \text{a.e. } x \in \mathcal{E}_h. \quad (4.1)$$

Next, we define the DG-norm related to the bilinear form (3.23).

**Definition 1** Define  $\| \cdot \|_\tau$ ,  $\tau \subset \partial\mathcal{K}$  as the (semi)-norm associated with the (semi)-inner-product

$$(v, w)_\tau = \int_\tau |B \cdot n| v w dS.$$

**Definition 2** Define the DG-norm  $\| \cdot \|_{DG}$  corresponding to the bilinear form (3.23) as

$$\begin{aligned} \|v\|_{DG}^2 &= \sum_{\mathcal{K} \in \mathcal{T}_h} \|D^{1/2} \bar{\nabla}_h v\|_{L^2(\mathcal{K})}^2 + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{D^n}^n} \|D^{1/2} \bar{r}_S(\llbracket v \rrbracket)\|_{L^2(\mathcal{E}_h)}^2 + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_M^n} \int_S \alpha(v^-)^2 dS \\ &+ \sum_{\mathcal{K} \in \mathcal{T}_h} \|c_0 v\|_{L^2(\mathcal{K})}^2 + \sum_{\mathcal{K} \in \mathcal{T}_h} \frac{1}{2} \|v^-\|_{\partial_+ \mathcal{K} \cap \Gamma_+}^2 + \sum_{\mathcal{K} \in \mathcal{T}_h} \frac{1}{2} \|v^-\|_{\partial_- \mathcal{K} \cap (\Gamma_- \cup \Gamma_D)}^2 \\ &+ \sum_{\mathcal{K} \in \mathcal{T}_h} \frac{1}{2} \|v^- - v^+\|_{\partial_- \mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)}^2. \end{aligned} \quad (4.2)$$

In following lemma we prove that the bilinear form (3.23) is coercive with respect to the DG-norm (4.2).

**Lemma 1** If  $\eta_0 > N_f$ , with  $N_f$  the number of faces of each element  $\mathcal{K} \in \mathcal{T}_h$ , then there exists a constant  $\beta > 0$ , independent of the meshsize  $h$ , such that

$$a(v, v) \geq \beta \|v\|_{DG}^2, \quad \forall v \in V_h.$$

*Proof.* First we substitute  $v$  for  $u_h$  in the bilinear forms (3.24b)-(3.24a) and use the fact that  $D$  is a symmetric positive definite matrix to obtain

$$a(v, v) = a_a(v, v) + a_d(v, v), \quad (4.3)$$

with

$$\begin{aligned}
a_a(v, v) &= \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} (-B \cdot \nabla_h v + cv) v d\mathcal{K} + \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial_+ \mathcal{K}} B \cdot n (v^-)^2 d\partial\mathcal{K} \\
&\quad + \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\partial_- \mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)} B \cdot n v^+ v^- d\partial\mathcal{K}, \\
a_d(v, v) &= \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} D^{1/2} \bar{\nabla}_h v \cdot D^{1/2} \bar{\nabla}_h v d\mathcal{K} - 2 \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{TD}^n} \int_S D^{1/2} \langle\langle v \rangle\rangle \cdot D^{1/2} \{ \bar{\nabla}_h v \} dS \\
&\quad + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_M^n} \int_S \alpha (v^-)^2 dS + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{TD}^n} \eta_0 \int_{\mathcal{E}_h} D^{1/2} \bar{r}_S(\llbracket v \rrbracket) \cdot D^{1/2} \bar{r}_S(\llbracket v \rrbracket) d\mathcal{K}.
\end{aligned}$$

For the proof of coercivity we first rewrite the bilinear form  $a_a(v, v)$ . Using the relation

$$(B \cdot \nabla_h v) v = \frac{1}{2} \nabla_h \cdot (B v^2) - \frac{1}{2} (\nabla_h \cdot B) v^2, \quad (4.4)$$

applying Gauss' Theorem and the boundary decomposition (3.21), for each element  $\mathcal{K} \in \mathcal{T}_h$  we have the relation

$$\begin{aligned}
&\int_{\mathcal{K}} (-B \cdot \nabla_h v + cv) v d\mathcal{K} + \int_{\partial_+ \mathcal{K}} B \cdot n (v^-)^2 d\partial\mathcal{K} + \int_{\partial_- \mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)} B \cdot n v^+ v^- d\partial\mathcal{K} \\
&= \int_{\mathcal{K}} \left( \frac{1}{2} \nabla_h \cdot B + c \right) v^2 d\mathcal{K} - \frac{1}{2} \int_{\partial\mathcal{K}} B \cdot n (v^-)^2 d\partial\mathcal{K} + \int_{\partial_+ \mathcal{K}} B \cdot n (v^-)^2 d\partial\mathcal{K} \\
&\quad + \int_{\partial_- \mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)} B \cdot n v^+ v^- d\partial\mathcal{K} \\
&= \int_{\mathcal{K}} \left( \frac{1}{2} \nabla_h \cdot B + c \right) v^2 d\mathcal{K} + \frac{1}{2} \int_{\partial_+ \mathcal{K} \cap \Gamma_+} B \cdot n (v^-)^2 d\partial\mathcal{K} + \frac{1}{2} \int_{\partial_+ \mathcal{K} \setminus \Gamma_+} B \cdot n (v^-)^2 d\partial\mathcal{K} \\
&\quad - \frac{1}{2} \int_{\partial_- \mathcal{K} \cap (\Gamma_- \cup \Gamma_D)} (B \cdot n) (v^-)^2 d\partial\mathcal{K} + \frac{1}{2} \int_{\partial_- \mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)} B \cdot n (v^-)^2 d\partial\mathcal{K} \\
&\quad - \int_{\partial_- \mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)} B \cdot n (v^- - v^+) v^- d\partial\mathcal{K}. \quad (4.5)
\end{aligned}$$

We have the relation

$$(v^- - v^+) v^- = \frac{1}{2} (v^-)^2 + \frac{1}{2} (v^- - v^+)^2 - \frac{1}{2} (v^+)^2, \quad (4.6a)$$

and due to cancellation of contributions of opposite sign, we also have

$$\sum_{\mathcal{K} \in \mathcal{T}_h} \frac{1}{2} \int_{\partial_+ \mathcal{K} \setminus \Gamma_+} B \cdot n (v^-)^2 d\partial\mathcal{K} + \sum_{\mathcal{K} \in \mathcal{T}_h} \frac{1}{2} \int_{\partial_- \mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)} B \cdot n (v^+)^2 d\partial\mathcal{K} = 0. \quad (4.6b)$$

If we introduce (4.6a)-(4.6b) into (4.5), we can write the bilinear form  $a_a(v, v)$  as

$$\begin{aligned}
a_a(v, v) &= \sum_{\mathcal{K} \in \mathcal{T}_h} \left( \int_{\mathcal{K}} \left( \frac{1}{2} \nabla_h \cdot B + c \right) v^2 d\mathcal{K} + \frac{1}{2} \int_{\partial_+ \mathcal{K} \cap \Gamma_+} B \cdot n (v^-)^2 d\partial\mathcal{K} \right. \\
&\quad \left. - \frac{1}{2} \int_{\partial_- \mathcal{K} \cap (\Gamma_- \cup \Gamma_D)} B \cdot n (v^-)^2 d\partial\mathcal{K} - \frac{1}{2} \int_{\partial_- \mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)} B \cdot n (v^- - v^+)^2 d\partial\mathcal{K} \right). \quad (4.7)
\end{aligned}$$

Using the boundary norm (Definition 1) and the conditions imposed on the function  $c_0$  (4.1), we have

$$\begin{aligned} a_a(v, v) &= \sum_{\mathcal{K} \in \mathcal{T}_h} \|c_0 v\|_{L^2(\mathcal{K})}^2 + \frac{1}{2} \sum_{\mathcal{K} \in \mathcal{T}_h} \|v^-\|_{\partial_+ \mathcal{K} \cap \Gamma_+}^2 + \frac{1}{2} \sum_{\mathcal{K} \in \mathcal{T}_h} \|v^-\|_{\partial_- \mathcal{K} \cap (\Gamma_- \cup \Gamma_D)}^2 \\ &\quad + \frac{1}{2} \sum_{\mathcal{K} \in \mathcal{T}_h} \|v^- - v^+\|_{\partial_- \mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)}^2. \end{aligned} \quad (4.8)$$

Next, we consider the bilinear form  $a_d(v, v)$ . Using the definition of the global lifting operator  $\bar{R}$ , which is the spatial part of the lifting operator  $R$  defined in (2.10b), we obtain

$$\begin{aligned} a_d(v, v) &= \sum_{\mathcal{K} \in \mathcal{T}_h} \|D^{1/2} \bar{\nabla}_h v\|_{L^2(\mathcal{K})}^2 + 2 \int_{\mathcal{E}_h} D^{1/2} \bar{\nabla}_h v \cdot D^{1/2} \bar{R}(\llbracket v \rrbracket) d\mathcal{K} \\ &\quad + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_M^n} \int_S \alpha(v^-)^2 dS + \eta_0 \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} \int_{\mathcal{E}_h} D^{1/2} \bar{r}_S(\llbracket v \rrbracket) \cdot D^{1/2} \bar{r}_S(\llbracket v \rrbracket) d\mathcal{K}. \end{aligned} \quad (4.9)$$

Using the Schwarz' inequality and the arithmetic-geometric mean inequality we obtain

$$-2 \int_{\mathcal{E}_h} D^{1/2} \bar{\nabla}_h v \cdot D^{1/2} \bar{R}(\llbracket v \rrbracket) d\mathcal{K} \leq \epsilon \|D^{1/2} \bar{\nabla}_h v\|_{L^2(\mathcal{E}_h)}^2 + \frac{1}{\epsilon} \|D^{1/2} \bar{R}(\llbracket v \rrbracket)\|_{L^2(\mathcal{E}_h)}^2, \quad (4.10a)$$

with  $\epsilon > 0$ , and

$$\|D^{1/2} \bar{R}(\llbracket v \rrbracket)\|_{L^2(\mathcal{E}_h)}^2 = \left\| \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} D^{1/2} \bar{r}_S(\llbracket v \rrbracket) \right\|_{L^2(\mathcal{E}_h)}^2 \leq N_f \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} \|D^{1/2} \bar{r}_S(\llbracket v \rrbracket)\|_{L^2(\mathcal{E}_h)}^2, \quad (4.10b)$$

with  $N_f$  the number of faces of each element  $\mathcal{K} \in \mathcal{T}_h$ . The relation (4.10b) is obtained as a consequence of relation (2.12), since the support of each  $r_S$  is the union of the element(s) sharing a face  $S \in \mathcal{S}_{ID}^n$  [2, 6]. Introducing (4.10a) and (4.10b) into (4.9) and combining with (4.8), we deduce

$$\begin{aligned} a(v, v) &\geq (1 - \epsilon) \sum_{\mathcal{K} \in \mathcal{T}_h} \|D^{1/2} \bar{\nabla}_h v\|_{L^2(\mathcal{K})}^2 + \left(\eta_0 - \frac{N_f}{\epsilon}\right) \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_{ID}^n} \|D^{1/2} \bar{r}_S(\llbracket v \rrbracket)\|_{L^2(\mathcal{E}_h)}^2 \\ &\quad + \sum_{n=0}^{N_t-1} \sum_{S \in \mathcal{S}_M^n} \int_S \alpha(v^-)^2 dS + \sum_{\mathcal{K} \in \mathcal{T}_h} \|c_0 v\|_{L^2(\mathcal{K})}^2 + \sum_{\mathcal{K} \in \mathcal{T}_h} \frac{1}{2} \|v^-\|_{\partial_+ \mathcal{K} \cap \Gamma_+}^2 \\ &\quad + \sum_{\mathcal{K} \in \mathcal{T}_h} \frac{1}{2} \|v^-\|_{\partial_- \mathcal{K} \cap (\Gamma_- \cup \Gamma_D)}^2 + \sum_{\mathcal{K} \in \mathcal{T}_h} \frac{1}{2} \|v^- - v^+\|_{\partial_- \mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)}^2, \end{aligned}$$

with  $\eta_0$  defined as  $\eta_0 = \min_{\mathcal{K} \in \mathcal{T}_h} \eta_{\mathcal{K}}$ . If we choose the parameters  $\eta_0 > N_f$  and  $\epsilon$  such that the relation  $\frac{N_f}{\eta_0} < \epsilon < 1$  holds, then for  $\beta = \min(1 - \epsilon, \eta_0 - \frac{N_f}{\epsilon})$  and  $\epsilon \in (0, 1)$ , we obtain the relation

$$a(v, v) \geq \beta \|v\|_{DG}^2,$$

which completes the proof of coercivity.  $\square$

**Theorem 1** *If  $\eta_0 > N_f$ , with  $N_f$  the number of faces of each element  $\mathcal{K} \in \mathcal{T}_h$ , then there exists a unique solution  $u_h \in V_h$  for the variational problem (3.25).*

*Proof.* To show the uniqueness of the DG solution for (3.25) it is sufficient to prove that the homogeneous equation:

Find a  $u_h \in V_h$  such that:

$$a(u_h, v) = 0, \quad \forall v \in V_h, \quad \text{with } u_h(t_0, \bar{x}) = 0, \quad (4.11)$$

only has the trivial solution  $u_h = 0$  for all  $t > t_0$ .

Assume  $u_h$  is a solution and choose  $v = u_h$  in the bilinear form  $a(u_h, v)$ . Then we rewrite the coercivity statement as:

$$\begin{aligned} a(u_h, u_h) &\geq \beta \|u_h\|_{DG}^2 = \beta \sum_{n=0}^{N_t-1} \left( \sum_{\mathcal{K} \in \mathcal{T}_h^n} \|D^{1/2} \bar{\nabla}_h u_h\|_{L^2(\mathcal{K})}^2 + \sum_{S \in \mathcal{S}_{ID}^n} \|D^{1/2} \bar{r}_S(\llbracket u_h \rrbracket)\|_{L^2(\mathcal{E}_h)}^2 \right. \\ &\quad + \sum_{S \in \mathcal{S}_M^n} \int_S \alpha (u_h^-)^2 dS + \sum_{\mathcal{K} \in \mathcal{T}_h^n} \|c_0 u_h\|_{L^2(\mathcal{K})}^2 \\ &\quad + \sum_{\mathcal{K} \in \mathcal{T}_h^n} \frac{1}{2} \|u_h^-\|_{\partial_+ \mathcal{K} \cap \Gamma_+}^2 + \sum_{\mathcal{K} \in \mathcal{T}_h^n} \frac{1}{2} \|u_h^-\|_{\partial_- \mathcal{K} \cap (\Gamma_- \cup \Gamma_D)}^2 \\ &\quad \left. + \sum_{\mathcal{K} \in \mathcal{T}_h^n} \frac{1}{2} \|u_h^- - u_h^+\|_{\partial_- \mathcal{K} \setminus (\Gamma_- \cup \Gamma_D)}^2 \right). \end{aligned} \quad (4.12)$$

First, consider the time slab for  $n = 0$ , then the coercivity condition in combination with  $u_h^+$  at  $t = 0$  implies  $u_h = 0$  in the first time slab. We can continue this argument to other time slabs and we obtain that  $u_h = 0$  is the only solution possible for the homogeneous equation. Hence the DG algorithm has a unique solution.  $\square$

## 5 Concluding Remarks

In this report we propose a new space-time DG method for the advection-diffusion-reaction equation. We derive the weak formulation and prove that the method gives a unique solution. The method is suitable for time-dependent domains. We will apply the method for the simulation of wet-chemical etching, where we solve a time-dependent advection-diffusion problem with a moving boundary. An a-posteriori error estimate for this method will also be a subject of future research.

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