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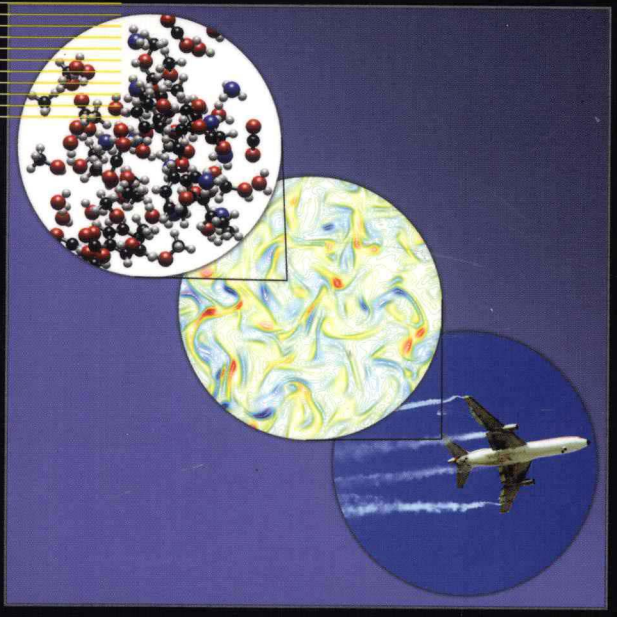

Björn Engquist
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Editors

Multiscale Methods in Science and Engineering

Springer

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With 85 Figures and 17 Tables

Springer

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Preface

Multiscale problems naturally pose severe challenges for computational science and engineering. The smaller scales must be well resolved over the range of the larger scales. Multiscale objects must therefore typically be described by a very large set of unknowns. The larger the ranges of scales, the more unknowns are needed and the higher the computational cost. It has been possible to meet many of these challenges by the recent progress in multiscale computational techniques coupled to the capability of the latest generation of computer systems.

This recent progress was presented at the conference *Multiscale Methods in Science and Engineering*, which was held in Uppsala, Sweden on January 26–28, 2004. More than 55 participants from six countries discussed the issues presented in the papers of this proceeding. The conference was sponsored by he Swedish Foundation for Strategic Research (SSF) and by the Swedish Agency for Innovation Systems, Vinnova via the Parallel and Scientific Computing Institute (PSCI).

Challenging multiscale problems are very common. One example can be average airflow, which typically depends on the details of small swirling eddies, which in turn depend on the interaction of molecules on much smaller scales in space and time. One can go further and see how the forces between the molecules depend on the electrons. Typically, a narrow range of scales is modeled by effective equations for that particular range. Turbulence models would then describe the coarsest scales of the phenomena mentioned above. The finer scales could be approximated by the Navies–Stokes equations, the Boltzmann equation and the Schrödinger equation respectively.

When such effective equations for a narrow range of scales can be derived the numerical approximations can be greatly facilitated. These equations should include the influence from other scales in the original multiscale problem. Techniques of this type are presented in this proceeding. In the contributions by Berlyand et al. and Svanstedt and Wellander, new variants of the homogenization technique are described and analyzed. Stochastic differential equations are increasingly common models for multiscale phenomena. New adaptive techniques for stochastic equations are developed by Dzougoutov et al. Stochastic models are also part of the systems studied by Jourdain et al. Sometimes there exist well performing equations for most

of the computational domain but a small subdomain contains microscales that are difficult to represent by the numerical method. Special subgrid models need to be developed. Edelvik derives such models for thin wires and slots in electromagnetic simulations. Thin filaments or fibers in fluids are approximated in the contribution by Tornberg. The latter simulations can also be seen as a way of numerically deriving effective equations for suspensions of filaments in fluids. The multiscale discontinuous Galerkin method studied by Aarnes and Heimsund uses multiscale basis functions and is based on homogenization theory.

An important preprocessing step for all numerical multiscale computations is the choice of unknowns. The number of these unknowns should be kept to a minimum. In the two contributions by Larson and collaborators this is achieved by adaptive grid generation based on realistic a posteriori estimates. Runborg uses a wavelet like technique that allows for a hierarchical and efficient representation of geometrical structures.

Computational multiscale methods are of two types. In the more established class of methods the full multiscale problem is discretized and highly efficient numerical methods are then applied to accurately compute the full range of scales. Multigrid, and the fast multipole method are very successful examples of such technique. These algorithms rely on special properties of the solution operator in order to achieve their optimal computational complexity. The smoothing by elliptic operators is one such example. Eberhard and Wittum presents a multigrid method for flow in heterogeneous porous media and a multipole method for electromagnetic scattering is described by Nilsson and Lötstedt.

In the second and more recent class of computational multiscale methods only a fraction of the microscale space is included in order to reduce the number of unknowns. The microscales and the macroscales are coupled in the same simulation exploiting special properties in the original problem, for example, scale separation. The simulation over a wide range of scales can be based on first principles even if effective equations are not known. The techniques discussed by E and Engquist, Jourdain et al., Samaey et al. and Sharp et al. in this proceeding are examples of this type of methods.

There are several active areas of development at the present time for tackling the multiscale challenge and many of the important ones were presented at this conference. The progress will have importance on the whole field of computational science and engineering. Multiscale modeling is emerging as a new computational paradigm.

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Contents

Multiscale Discontinuous Galerkin Methods for Elliptic Problems with Multiple Scales

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Summary. We introduce a new class of discontinuous Galerkin (DG) methods for solving elliptic problems with multiple scales arising from e.g., composite materials and flows in porous media. The proposed methods may be seen as a generalization of the multiscale finite element (FE) methods. In fact, the proposed DG methods are derived by combining the approximation spaces for the multiscale FE methods and relaxing the continuity constraints at the inter-element interfaces. We demonstrate the performance of the proposed DG methods through numerical comparisons with the multiscale FE methods for elliptic problems in two dimensions.

Key words: multiscale methods, discontinuous Galerkin methods, elliptic partial differential equations

1 Introduction

We consider solving the second-order elliptic equation

$$\begin{cases} -\nabla \cdot (a(x)\nabla u) = f, & \text{in } \Omega \subset \mathcal{R}^{\mathrm{d}}, \\ u = 0, & \text{on } \Gamma_{\mathrm{D}} \subset \partial\Omega, \\ -a(x)\nabla u \cdot n = 0, & \text{on } \Gamma_{\mathrm{N}} = \partial\Omega \backslash \Gamma_{\mathrm{D}}, \end{cases} \tag{1}$$

where Ω is bounded, $\partial\Omega$ is Lipschitz, n is the outward unit normal on $\partial\Omega$ and $a(x) = (a_{ij}(x))$ is a symmetric positive definite tensor with uniform upper and lower bounds:

$$0 < \alpha|y|^2 \leq y^T a(x) y \leq \beta|y|^2 < \infty, \quad \forall x \in \Omega,\ \forall y \in \mathcal{R}^d,\ y \neq 0.$$

We will interpret the variable u as the (flow) potential and q as the (flow) velocity. The homogeneous boundary conditions are chosen for presentational brevity. General boundary conditions can be handled without difficulty.

Equation (1) may represent incompressible single-phase porous media flow or steady state heat conduction through a composite material. In single-phase flow, u

is the flow potential, $q = -a(x)\nabla u$ is the Darcy filtration velocity and $a(x)$ is the (rock) permeability of the porous medium. For heat conduction in composite materials, u, q and $a(x)$ represents temperature, heat flow density, and thermal conductivity respectively. These are typical examples of problems where $a(x)$ can be highly oscillatory and the solution of (1) displays a multiscale structure. This leads to some fundamental difficulties in the development of robust and reliable numerical models.

In this paper we introduce a new class of DG methods for solving this particular type of multiscale elliptic problems. Until recently, DG methods have been used mainly for solving partial differential equations of hyperbolic type, see e.g. [10] for a comprehensive survey of DG methods for convection dominated problems. Indeed, whereas DG methods for hyperbolic problems have been subject to active research since the early seventies, it is only during the last decade or so that DG methods have been applied to purely elliptic problems, cf. [5] and the references therein. The primary motivation for applying DG methods to elliptic problems is perhaps their flexibility in approximating rough solutions that may occur in elliptic problems arising from heterogeneous and anisotropic materials. However, to our knowledge, previous research on DG methods for elliptic problems has been confined to solving elliptic partial differential equations with smooth coefficients.

DG methods approximate the solution to partial differential equations in finite dimensional spaces spanned by piecewise polynomial base functions. As such, they resemble the FE methods, but, unlike the FE methods, no continuity constraints are explicitly imposed at the inter-element interfaces. This implies that the weak formulation subject to discretization must include jump terms across interfaces and that some artificial penalty terms must be added to control the jump terms. On the other hand, the weak continuity constraints give DG methods a flexibility which allows a simple treatment of, e.g., unstructured meshes, curved boundaries and h- and p-adaptivity. Another key feature with DG methods is their natural ability to impose mass conservation locally. Moreover, the "local" formulation of the discrete equations allows us us to use grid cells of arbitrary shapes without difficulty. We may therefore choose the gridlines to be aligned with sharp contrasts in, for instance, underlying heterogeneous materials.

The multiscale FE methods (MsFEMs) introduced in [9, 12] have been successfully applied to multiscale elliptic problems, but their accuracy is to some degree sensitive to the selection of the boundary conditions that determine the FE base functions. If, for instance, strong heterogeneous features penetrate the inter-cell interfaces, then simple, e.g. linear, boundary conditions may be inadequate. In such situations, oversampling strategies or other techniques for the generation of adaptive boundary conditions must be used to recover the desired order of accuracy. This sensitivity to the selection of boundary conditions is partly due to the strong continuity requirements at the inter-element interfaces implicit in the FE methods.

Here we propose a class of multiscale DG methods (MsDGMs) for solving elliptic problems with multiple scales. One of the primary motives for developing MsDGMs is to generate multiscale methods that are less sensitive to the selection of boundary conditions for the base functions than is the case for the MsFEMs. Another nice feature with MsDGMs is that they produce solutions for both the potential

variable (e.g. pressure or temperature) and the velocity variable (e.g. phase velocity or thermal flux density) that reflect important subgrid variations in the elliptic coefficients. We will demonstrate the benefit of using multiscale methods in comparison with ordinary monoscale numerical methods and perform numerical experiments to display the performance of the MsDGMs relative to the original and mixed MsFEMs. We therefore attempt to reveal that there is a need for multiscale methods, and to demonstrate under what circumstances it may be advantageous to relax the inter-element continuity assumptions implicit in the MsFEMs.

The paper is organized as follows. We give the general mathematical setting for the DG methods in Sect. 2 and show how they are related to the more familiar FE methods. In particular we show that both standard and mixed FE methods may be viewed as special DG methods. This observation allows us to extend this type of FE methods to corresponding DG methods. In Sect. 3 we outline the MsFEMs introduced in [12] and [9] and exploit the relationship between FE methods and DG methods to derive a corresponding class of MsDGMs. Finally, Sect. 4 contains the numerical experiments and we conclude with a discussion of the results in Sect. 5.

2 Mathematical Formulations

In Sect. 2.1 we give the mathematical formulation of the DG methods for (1) and discuss the selection of the so-called numerical fluxes that are used to force weak continuity of the solution across inter-element interfaces. In Sect. 2.2 we show how the conforming and mixed FE methods may be viewed as special DG methods, and describe how such FE methods can be extended to corresponding DG methods.

2.1 Discontinuous Galerkin Methods

To define the DG methods we split (1) into the first order system,

$$\begin{aligned} q &= -a(x)\nabla u, && \text{in } \Omega, \\ \nabla \cdot q &= f, && \text{in } \Omega, \\ u &= 0, && \text{on } \Gamma_{\mathrm{D}}, \\ q \cdot n &= 0, && \text{on } \Gamma_{\mathrm{N}}. \end{aligned}$$

Furthermore, define the following approximation spaces:

$$\begin{aligned} Q_N &= \{p \in (H^1(\Omega))^d : p \cdot n = 0 \text{ on } \Gamma_N\}, \\ U_D &= \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma_D\}. \end{aligned}$$

Upon integration by parts, we now deduce the weak formulation: Find $q \in Q_N$ and $u \in U_D$ such that

$$\int_\Omega a^{-1} q \cdot p \, \mathrm{d}x = \int_\Omega u \nabla \cdot p \, \mathrm{d}x \qquad \forall p \in Q_N,$$

$$\int_\Omega q \cdot \nabla v \, \mathrm{d}x = -\int_\Omega f v \, \mathrm{d}x \qquad \forall v \in U_D.$$

In the DG methods, a similar set of equations is derived for each grid cell. However, for the grid cell equations it is not natural to impose homogeneous boundary conditions. The boundary conditions are therefore approximated from neighboring values of the unknown solution. Essentially we want to ensure that the potential u and the velocity q are "almost" continuous at the interfaces. Since we do not want to enforce continuity by imposing constraints on the approximation spaces as the FE methods do, we have to penalize the deviation from continuity by introducing an artificial penalty term. To understand the mechanism behind the penalty term, we digress for a moment in order to consider an example that illustrates the basic principle.

Example: Consider the Poisson equation with Dirichlet data,

$$\begin{cases} -\Delta u = f, \text{ in } \Omega, \\ u = g, \text{ on } \partial\Omega, \end{cases}$$

and for each $\epsilon > 0$, let $u_\epsilon \in H^1(\Omega)$ be the solution to the regularized problem

$$\int_\Omega \nabla u_\epsilon \cdot \nabla v \,\mathrm{d}x + \int_{\partial\Omega} \frac{1}{\epsilon}(u_\epsilon - g)v \,\mathrm{d}s = \int_\Omega fv \,\mathrm{d}x \quad \forall v \in H^1(\Omega). \tag{2}$$

Here ds denotes the surface area measure. This problem corresponds to perturbing the boundary data so that instead of $u = g$ we have $u + \epsilon\nabla u \cdot n = g$ on $\partial\Omega$. One can show that (2) is well posed and that $u_\epsilon \to u \in H_0^1(\Omega)$ as $\epsilon \to 0$ [14]. Hence, we see that the extra penalty term is added in order to force, in the limit $\epsilon \to 0$, the satisfaction of the boundary conditions.

Just as the satisfaction of the Dirichlet boundary data was imposed weakly in (2), so can inter-element continuity be attained in a similar fashion. It was this observation that originally led to the development of the interior penalty (IP) methods [4, 11, 16]. Arnold et al. [5] recently recognized that the IP methods, along with several other methods with discontinuous approximation spaces, can be classified as DG methods. These methods differ in the flux approximating schemes used to force continuity at the inter element interfaces. We now describe the general framework for the DG methods with respect to the elliptic problem (1).

Let $\mathcal{T}(\Omega) = \{T \in \mathcal{T}\}$ be a family of elements in a partitioning of Ω and define $\partial\mathcal{T} = \cup\{\partial T : T \in \mathcal{T}\}$, $\Gamma = \partial\mathcal{T}\backslash\partial\Omega$ and $\Gamma_{ij} = \partial T_i \cap \partial T_j$, $T_i, T_j \in \mathcal{T}$. Next, introduce an approximation space $Q^h \times U^h \subset (H^1(\mathcal{T}))^d \times H^1(\mathcal{T})$ where

$$H^k(\mathcal{T}) = \{w \in L^2(\Omega) : w \in H^k(T), \forall T \in \mathcal{T}\}.$$

The DG method then seeks $q^h \in Q_N^h = Q^h \cap Q_N$ and $u^h \in U_D^h = U^h \cap U_D$ such that

$$\int_T a^{-1} q^h \cdot p \,\mathrm{d}x = \int_T u^h \nabla \cdot p \,\mathrm{d}x - \int_{\partial T} \bar{u}\, p \cdot n_T \,\mathrm{d}s \qquad \forall p \in Q_N^h, \tag{3}$$

$$\int_T q^h \cdot \nabla v \,\mathrm{d}x = -\int_T fv \,\mathrm{d}x + \int_{\partial T} v\, \bar{q} \cdot n_T \,\mathrm{d}s \qquad \forall v \in U_D^h, \tag{4}$$

for all $T \in \mathcal{T}$. Here n_T is the outward unit normal on ∂T and $(\bar{q}, \bar{u})$ are the so called numerical fluxes which represent an approximation to (q, u) on ∂T.

The Numerical Fluxes

The perhaps simplest and most natural choice of numerical fluxes is to set

$$(\bar{q}, \bar{u}) = \frac{1}{2}\left[(q^h, u^h)|_{T_i} + (q^h, u^h)|_{T_j}\right] \quad \text{on } \Gamma_{ij}.$$

We see that this option, which was considered by Bassi and Rebay in [6], does not involve a penalty term and simply computes the fluxes by taking the average of the functional limits on each side of the inter-element interfaces Γ_{ij}. Though this option seems attractive, the lack of a penalty term renders the method unstable and may lead to a singular discretization matrix on certain grids. It is therefore clear that the stabilization of the DG methods via the inclusion of a penalty term is crucial. In fact, without it, not only stability is affected, but convergence is degraded or lost [5].

To define the numerical fluxes that will be used in this paper, it is convenient to introduce, for $q \in Q^h$, $u \in U^h$, and $x \in \Gamma_{ij}$, the mean value operators

$$\{u\}(x) = \frac{1}{2}(u_i(x) + u_j(x)),$$
$$\{q\}(x) = \frac{1}{2}(q_i(x) + q_j(x)),$$

and the associated jump operators

$$[u](x) = \frac{1}{2}(u_i(x) - u_j(x))n_{ij},$$
$$[q](x) = \frac{1}{2}(q_i(x) - q_j(x)) \cdot n_{ij}.$$

Here $(q_k, u_k) = (q, u)|_{T_k}$ and n_{ij} is the unit normal on Γ_{ij} pointing from T_i to T_j. We shall employ the numerical fluxes associated with the method of Brezzi et al. [7], which are

$$\bar{u} = \{u^h\}, \quad \bar{q} = \{q^h\} - \eta[u^h]. \tag{5}$$

These numerical fluxes have been analyzed in [8] in the wider context of LDG (Local Discontinuous Galerkin) methods, and gives a stable, convergent method when $\eta = \mathcal{O}(1/h)$. While there are many other numerical fluxes that has been proposed for DG methods, see e.g., [5], we have chosen to use the Brezzi fluxes (5) because they are simple, stable, and consistent, and give the same rate of convergence (at least for elliptic problems with smooth coefficients) as more elaborate DG methods.

The Primal Formulation

The need to construct approximation spaces for both the potential variable and the velocity variable leads to a relatively large number of degrees of freedom per element. However, it is standard procedure in the literature on DG methods to eliminate

the velocity variable from the discretized equations. This elimination leads to the primal formulation:

$$B^h(u^h, v) = \int_\Omega fv \, \mathrm{d}x, \quad \forall v \in U^h, \tag{6}$$

where the primal form $B^h(\cdot,\cdot)$ is defined by

$$\begin{aligned} B^h(u^h, v) := \textstyle\int_\Omega \nabla u^h \cdot a \nabla v \, \mathrm{d}x + \int_{\partial\mathcal{T}} ([\bar{u} - u^h] \cdot \{a\nabla v\} + \{\bar{q}\} \cdot [v]) \, \mathrm{d}s \\ + \textstyle\int_{\partial\mathcal{T}\setminus\partial\Omega} (\{\bar{u} - u^h\}[a\nabla v] + [\bar{q}]\{v\}) \, \mathrm{d}s, \end{aligned} \tag{7}$$

and $\bar{q} = \bar{q}(u^h, q^h)$ is defined with the understanding that q^h satisfies

$$\begin{aligned} -\textstyle\int_\Omega a^{-1} q^h \cdot p \, \mathrm{d}x = \int_\Omega \nabla u^h \cdot p \, \mathrm{d}x + \int_{\partial\mathcal{T}} [\bar{u} - u^h] \cdot \{p\} \, \mathrm{d}s \\ + \textstyle\int_{\partial\mathcal{T}\setminus\partial\Omega} \{\bar{u} - u^h\}[p] \, \mathrm{d}s. \end{aligned} \tag{8}$$

If the unknowns associated with the velocity variable q^h are numbered sequentially, element by element, then the matrix block that stems from the term on the left hand side of (8) becomes block diagonal. This allows us to perform a Schur-elimination of the discretization matrix to give the reduced form corresponding to $B^h(\cdot,\cdot)$ at a low cost. Thus, to compute u^h using the primal formulation, we eliminate first the velocity variable by Schur-elimination. The next step is to solve (6) for u^h. Finally one obtains an explicit expression for the fluxes by back-solving for q^h in (8).

For the numerical fluxes considered in this paper, we have $\bar{u} = \{u^h\}$. Thus, since $\bar{q}$ is conservative, i.e., unit valued on $\partial\mathcal{T}$, the integral over $\partial\mathcal{T}\setminus\partial\Omega$ in $B^h(u^h, v)$ vanishes, and the primal form reduces to

$$B^h(u^h, v) := \int_\Omega \nabla u^h \cdot a \nabla v \, \mathrm{d}x - \int_{\partial\mathcal{T}} ([u^h] \cdot \{a\nabla v\} - \{\bar{q}\} \cdot [v]) \, \mathrm{d}s. \tag{9}$$

Finally, inserting $\bar{q} = \{q^h\} - \eta[u^h]$ into (9) gives

$$B^h(u^h, v) = \int_\Omega \nabla u^h \cdot a \nabla v \, \mathrm{d}x - \int_{\partial\mathcal{T}} [u^h] \cdot \{a\nabla v\} - (\{q^h\} - \eta[u^h]) \cdot [v] \, \mathrm{d}s. \tag{10}$$

A rigorous analysis of the primal form (10) in the case of polynomial elements can be found in [5]. There it was shown that the bilinear form (10) is bounded and stable, provided that the stabilizing coefficient η is chosen sufficiently large. Hence, the same type of constraint applies to η either we formulate the DG method using the mixed formulation (3)–(4) or the primal formulation (6) and (8) using the primal form (10).

2.2 Finite Element Methods vs. Discontinuous Galerkin Methods

The standard conforming FE discretization of (1) approximates the solution in a finite dimensional subspace V^h of $H^1(\Omega)$. Though $H^1(\Omega)$ is not in general embedded in

$C(\bar{\Omega})$, the discrete FE approximation spaces are. This implies in particular that the corresponding FE methods approximates a possible irregular solution with a continuous one. This continuity assumption can be relaxed, as the non-conforming FE methods do, but they still restrain the solution by putting explicit restrictions on the approximation space. This is in a sense the main difference between FE methods and the DG methods which impose continuity implicitly in a weak sense.

In order to clarify the differences, or perhaps rather the similarities, between FE methods and DG methods for equation (1), we first review the concept behind FE methods. In the standard FE formulation of (1) we define a finite dimensional subspace $U^h \subset H^1(\Omega) \cap C(\bar{\Omega})$ and seek $u \in U_D^h(\Omega) = \{u \in U^h : u = 0 \text{ on } \Gamma_D\}$ such that

$$\int_\Omega (\nabla u^h)^T a \nabla v \, \mathrm{d}x = \int_\Omega f v \, \mathrm{d}x \quad \forall v \in U_D^h.$$

Now, since $U^h \subset C(\bar{\Omega})$ we know that u^h is continuous. Hence, it makes sense to let $\bar{u} = u^h$ in (7). We then deduce that the primal form (7) reduces to

$$B^h(u^h, v) = \int_\Omega (\nabla u^h)^T a \nabla v \, \mathrm{d}x + \int_{\partial \mathcal{T} \setminus \Omega} [\bar{q}]\{v\}. \tag{11}$$

Thus, if the numerical flux $\bar{q}$ is conservative, i.e. if $\bar{q}$ is single valued on $\partial \mathcal{T} \setminus \Omega$, then the last term on the right hand side of (11) vanishes. Thus, for any approximation space Q^h, the primal formulation of DG methods with a conservative numerical flux for the velocity variable and an approximation space $U^h \subset C(\bar{\Omega})$ reduces to the standard FE variational formulation.

Similarly, in mixed FE methods one seeks a solution (q^h, u^h) of the elliptic problem (1) in a finite dimensional subspace $Q_N^h \times U_D^h$ of $H(\mathrm{div}, \Omega) \times \mathrm{L}^2(\Omega)$. The subscripts N and D indicate that functions in Q_N^h and U_D^h satisfy the homogeneous Neumann and Dirichlet conditions on Γ_N and Γ_D respectively. The mixed FE solution is defined by the following mixed formulation:

$$\begin{aligned} \int_\Omega a^{-1} q^h \cdot p \, \mathrm{d}x &= \int_\Omega u^h \nabla \cdot p \, \mathrm{d}x, && \forall p \in Q_N^h, \\ \int_\Omega \nabla \cdot q^h v \, \mathrm{d}x &= \int_\Omega f v \, \mathrm{d}x, && \forall v \in U^h, \end{aligned}$$

where n is the outward unit normal on $\partial\Omega$.

For many standard mixed FE methods for equation (1), such as the Raviart–Thomas method [15], the approximation space for the velocity consists of functions that are continuous across the interfaces Γ_{ij} in the direction of the coordinate unit normal n_{ij}. For this type of methods we have $\int_{\Gamma_{ij}} [q] ds = 0$ for all $\Gamma_{ij} \subset \Gamma$ and $q \in Q^h$. Thus, by setting $\bar{q} = q^h$ on Γ and $\bar{q} \cdot n = 0$ on Γ_N we find that the second equation above transforms, upon integration by parts, to equation (4). Moreover, if the numerical flux $\bar{u}$ for the potential is single-valued on Γ, then the first equation in the mixed formulation coincides with equation (3). This shows that also mixed FE methods for equation (1) can be viewed as special DG methods for which the numerical fluxes are determined by continuity conditions imposed on the approximation