An Unfitted Discontinuous Galerkin Finite Element Method for Pore Scale Simulations

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Abstract. Groundwater processes are always multi scale processes. The understanding of the pore scale is important in order to understand the system as a whole.
Handling the pore scale in a numerical simulation is not easy. The solid phase forms a complex shaped geometry and for multiscale simulations a good approximation of this geometrical shape is crucial to obtain reliable numerical results, while the interest on the other hand lies only in a coarse solution, which would allow a smaller number of unknowns.
A new discretization scheme for solving PDEs in complex domains was developed. It combines the idea of Unfitted Finite Elements with a Discontinuous Galerkin (DG) Finite Elements discretization. It will be shown how this approach can be used for numerical upscaling. This allows a more efficient estimation of parameters on the continuum scale from pore scale processes.

Key words: Discontinuous Galerkin, Finite Elements, Multiscale Simulations, Numerical Upscaling, C++, Generic Programming

1 Multiscale Character of Groundwater Processes

When discussing groundwater processes the soil structure must be taken into account. Soil does not form a homogeneous material, but exhibits an extensive multiscale structure. Heterogeneities are visible at all scales, down to the pore scale.

On the pore scale groundwater flow is described by Navier-Stokes equation through a complicated shaped domain. Fluid velocity in groundwater processes are usually slow, therefore the flow can be assumed to be laminar and the nonlinear Navier term can be neglected. The governing equation is then the Stokes Equation:

$$\begin{aligned} -\mu\Delta\mathbf{u} + \nabla p &= \mathbf{f} && \text{in} && \Omega \subset \mathbb{R}^3 \\ \nabla\cdot\mathbf{u} &= 0 && \text{in} && \Omega \\ \mathbf{u} &= 0 && \text{on} && \Gamma_0 \subseteq \partial\Omega \\ \mathbf{u}\cdot\hat{\mathbf{n}} &= u && \text{on} && \Gamma_N \subseteq \partial\Omega \setminus \Gamma_0 \\ \partial_n\mathbf{u} + p &= p_0 && \text{on} && \Gamma_P = \partial\Omega \setminus (\Gamma_0 \cup \Gamma_N)\,, \end{aligned} \tag{1}$$

with the viscosity μ, the velocity $\mathbf{u}$ and the pressure p. On the internal boundaries, the surface of the grains, no-slip boundary conditions are appropriate. On the macroscopic boundaries, one may choose between Dirichlet like flux boundary conditions and pressure boundary conditions.

On the macroscopic scale groundwater flow is described by an empirical flux law introduced in [1]. It is usually referred to as *Darcy's Law*:

$$\begin{aligned} \nabla \cdot \mathbf{j} &= 0 && \text{in} \quad \Omega \subset \mathbb{R}^3 \\ \mathbf{j} &= -\tfrac{1}{\mu} \underline{\kappa} \nabla p && \text{in} \quad \Omega \\ p &= p_0 && \text{on} \quad \Gamma_D \subseteq \partial\Omega \\ \mathbf{j} \cdot \hat{\mathbf{n}} &= j && \text{on} \quad \Gamma_N = \partial\Omega \setminus \Gamma_D \,, \end{aligned} \tag{2}$$

where $\mathbf{j}$ denotes the flux, $\hat{\mathbf{n}}$ is the outwards pointing normal vector, p the pressure, μ the viscosity and $\underline{\kappa}$ the permeability tensor. In numerical simulations, $\underline{\kappa}$ often is assumed to be a diagonal tensor.

The pore velocity $\mathbf{u}$ is given by the flux $\mathbf{j}$ and the porosity ρ

$$\mathbf{u} = \frac{\mathbf{j}}{\rho} \,. \tag{3}$$

2 Unfitted Discontinuous Galerkin Method

1987 [2] presented a discretization method on an unfitted mesh, using conforming finite element methods. The finite element mesh does not resolve the geometry. Boundary conditions along the geometry are enforced weakly using Nitsche's method [3]. However, the method itself does only allow first order trial and test functions. Also methods using first order Lagrange shape functions are not mass conservative.

We extended this approach using Discontinuous Galerkin methods [4]. This allows higher order computations. Furthermore for both, Stokes Equation and Darcy's law, locally mass conservative Discontinuous Galerkin discretizations do exist.

Given a domain $\Omega \subseteq \mathbb{R}^d$, $\mathcal{G}$ is a disjoint partitioning of Ω into sub-domains

$$\mathcal{G}(\Omega) = \left\{ \Omega^{(0)}, \ldots, \Omega^{(N-1)} \right\} . \tag{4}$$

The partitioning $\mathcal{G}$ is usually based on geometrical properties and the boundaries $\partial\Omega^{(i)}$ may have a complex shape. On a sub-domain $\Omega^{(i)}$ we want to solve a partial differential equation together with suitable boundary conditions.

The finite element mesh for $\Omega^{(i)}$ is constructed, using the triangulation

$$\mathcal{T}(\Omega) = \{E_0, \ldots, E_{M-1}\} \,. \tag{5}$$

Based on (5) the triangulation $\mathcal{T}(\Omega^{(i)})$ is defined

$$\mathcal{T}(\Omega^{(i)}) = \left\{ E_n^{(i)} = \Omega^{(i)} \cap E_n \;\middle|\; E_n^{(i)} \neq \emptyset \right\} . \tag{6}$$

Note that the elements $E^{(i)}$ can be arbitrarily shaped and in general will not be convex.

On the fundamental element E_n $\varphi_{n,j} \in P_k$ denotes a polynomial, where P_k is the space of polynomial functions of degree k. The shape functions $\varphi_{n,j}^{(i)}$ are given by polynomials $\varphi_{n,j} \in P_k$ with their support restricted to $E_n^{(i)} \in \mathcal{T}(\Omega^{(i)})$.

The resulting finite element space is defined by

$$V_k^{(i)} = \left\{ v \in L_2(\Omega^{(i)}) \;\middle|\; v|_{E_n^{(i)}} \in P_k \right\} \tag{7}$$

and is discontinuous on the internal skeleton.

For the discretization of the Stokes equation we are using the Discontinuous Galerkin formulation described in [5]. The discretization leads to a problem that reads: Find $\mathbf{u} \in {V_k^{(i)}}^3$, $p \in V_{k-1}^{(i)}$ such that

$$\begin{aligned} a(\mathbf{u},\mathbf{v}) + J(\mathbf{u},\mathbf{v}) + b(\mathbf{v},p) &= l(\mathbf{v}) \qquad && \forall\ \mathbf{v} \in {V_k^{(i)}}^3 \quad , \\ b(\mathbf{u},q) &= 0 && \forall\ q \in V_{k-1}^{(i)} \quad . \end{aligned} \tag{8}$$

$J(\mathbf{u},\mathbf{v})$ is a penalty term, there is no physical equivalent to this term. It vanishes for $h \to 0$ and penalizes jumps in the solution, in order to enforce a certain continuity of the solution. Dirichlet type boundary conditions (e.g. no-slip and no-flux) are enforced weakly.

This discretization will then require the evaluation of integrals on these arbitrary shaped elements $E^{(i)}$ and on their surface $\partial E^{(i)}$.

3 Multiscale Simulations

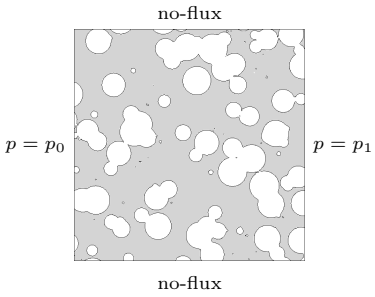

Fig. 1. A macroscopic pressure gradient is imposed along the x axis using pressure boundary conditions and no-flux boundary condition are applied on the all other macroscopic boundaries. Micro scale computations with no-slip boundary condition on the grain surface yield an effective κ_{xx}.

Given a domain Ω, the form of a cube, $\mathcal{G}$ describes a partition of Ω into void space Ω^v and pore space Ω^p (see Fig. 3). Assuming Ω to be the size of an

REV (Representative Elementary Volume; [6]), effective parameters for Darcy's Law on this REV can be computed solving Stokes Equation on the pore space domain Ω^p.

We impose a pressure gradient ∇p along one of the coordinate axis as pressure boundary condition for (1). On all inner boundaries $\partial\Omega^p \setminus \partial\Omega$ no-slip boundary condition is imposed.

The mean velocity

$$\bar{\mathbf{u}} = \int_{\Omega^p} \mathbf{u} dx \cdot |\Omega^p|^{-1} \tag{9}$$

and the macroscopic porosity $\bar{\rho} = \frac{|\Omega^p|}{|\Omega|}$ yield an effective permeability

$$\kappa_{xx} = -\frac{\mathbf{u}\rho}{\nabla p} \ . \tag{10}$$

$|\Omega|$ denotes the size of Ω.

4 Implementation

The presented computations are implemented in a generalized framework work Discontinuous Galerkin Methods on unfitted meshes. It is built onto the DUNE framework [7, 8]. DUNE is a generic C++ toolbox for grid based methods. The current results were computed sequentially, but design of the method and the way it is building on the DUNE interface enables an easy future parallalization.

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