Simulating Structure Formation in Soils across Scales using Discontinuous Galerkin Methods

Simulation von Strukturbildung im Boden auf unterschiedlichen Skalen mithilfe unstetiger Galerkin–Verfahren

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Simulation von Strukturbildung im Boden auf unterschiedlichen Skalen mithilfe unstetiger Galerkin–Verfahren

Zusammenfassung

Darüber hinaus sollen Effekte der aus dem Modell gewonnenen Erkenntnisse auf für Anwender relevantere Skalen übertragen werden. Die Qualitätsbeurteilung entsprechender gemittelten Modelle für etwa die Feldskala ist von allgemeinem Interesse, da Simulationen, welche die Geometrie der verschiedenen Mikroaggregate auf der Mikroskala auflösen, unter ökonomischen Gesichtspunkten nicht praktikabel sind. Deshalb werden in dieser Dissertation verschiedene Parametrisierungen für Diffusivitäten mit rigoros hergeleiteten Resultaten verglichen und Vorschläge für Verbesserungen der Formeln gemacht, die in einschlägiger Literatur zu finden sind.

Aus mathematischer Sicht resultiert ein Problem aus der Tatsache, dass sich die Geometrie des Modells auf der Mikroskala diskret bewegt. Es stellt sich die Frage, ob entsprechende gemittelte Größen auch wirklich in Modellen auf anderen Skalen verwendet werden können oder ob deren Lösungen wiederum durch den artifiziellen zeitlichen Sprung in den Parametern zu sehr verfälscht werden. Auch dieser Aspekt wird im Folgenden behandelt und die Verlässlichkeit gewonnener Parameter unterstrichen.


**Aufbau der Arbeit nach Kapiteln**


Kapitel 3 behandelt die Homogenisierung von Diffusionsprozessen in porösen Medien. Hier werden zunächst einige bekannte Formeln, die einen funktionalen Zusammenhang zwischen der Diffusivität und der Porosität eines porösen
Mediums herstellen, verglichen. Danach werden diese Formeln mit mathema-
tisch rigorosen Ausdrücken für spezielle Mikrostrukturen in Beziehung gesetzt. Im Anschluss werden die numerischen Methoden vorgestellt, mit denen Zu-
sammenhänge zwischen der Diffusion auf der einen Seite und der Porosität, der Oberfläche der soliden Matrix und der Tortuosität auf der anderen Seite hergestellt werden.

Kapitel 4 behandelt die Frage, ob es gerechtfertigt ist Tensoren — die aus einem zeitlich diskreten Mikromodell abgeleitet sind — für ein zeitlich kon-
tinuierliches Makromodell zu verwenden. Hierzu wird zunächst ein Problem untersucht, bei dem davon ausgegangen wird, dass höchstens abzählbar un-
endlich viele Sprünge auftreten. Obwohl dies der für unser Modell relevante Fall ist wird weitergehend formal untersucht, ob man eine Formel finden kann, die einen zeitlich oszillierenden Tensor homogenisiert (ähnlich wie sonst bei örtlich oszillierenden Tensoren).

Die Untersuchung des verwendeten numerischen Verfahrens befindet sich in Kapitel 5. Hier wird die „local discontinuous Galerkin“ Methode zunächst auf eine partielle Differentialgleichung angewendet, die im Modell aus Kapi-
tel 2 vorkommt. Hierbei handelt es sich um eine Diffusionsgleichung mit einer Sprungbedingung, wie sie zum Beispiel durch das Henry Gesetz beschrieben wird. Es werden Stabilität und Konvergenz des Verfahrens für die eben beschrie-
bene Gleichung gezeigt und die Verwendung von Ansatzräumen mit verschie-
denen polynomiellen Ordnungen für die primäre und die sekundäre Variable empfohlen, da diese analytisch und numerisch das gleiche Konvergenzverhalten zeigen, aber den Rechenaufwand deutlich reduzieren. Die allgemeine Anwend-
barkeit dieser mathematischen Neuerung wird weiter durch die Anwendung des Verfahrens auf die nicht-lineare Advektions–Diffusions–Gleichung gezeigt, bei der ebenfalls eine Reduktion des Rechenaufwands bei gleichem Konver-
genverhalten festgestellt wird. Zuletzt werden die erzielten Ergebnisse auf eine hybridisierte Form des Verfahrens übertragen.

Die vorliegende Arbeit wird mit einigen Kommentaren und einem Ausblick auf mögliche weitere Forschungsaspekte in Kapitel 6 geschlossen.

Bereits publizierte Beiträge
Weite Teile der vorliegenden Promotionsschrift konnten bereits in Form von Manuskripten veröffentlicht werden. Diese Artikel sind:

[1] V. Aizinger, A. Rupp, J. Schütz und P. Knabner. „Analysis of a mixed discontinuous Galerkin method for instationary Darcy flow“. *Computa-
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Zusammenfassung (German)


Abschnitt 5.3 ist in Zusammenarbeit mit Vadym Aizinger, Balthasar Reuter und Peter Knabner entstanden. Vadym Aizinger und Peter Knabner haben im Rahmen ihrer Betreuungstätigkeiten an diesem Abschnitt Anteil. Andreas Rupps Anteil besteht in der Analysis und Balthasar Reuters Anteil in der numerischen Umsetzung der Methode.

Abschnitt 5.4 entstammt der Master–Arbeit von Markus Musch, die von An-
dreas Rupp betreut wurde. Der Abschnitt ist in sehr ähnlicher Form als Manuskript zur Begutachtung bei einem wissenschaftlichen Journal eingereicht.

Neben den oben genannten Veröffentlichungen ist Andreas Rupp Koautor von


Diese vier Artikel werden aber in der vorliegenden Monographie nicht verwendet.
Chapter 1

Introduction

This thesis deals with mathematical modeling, analysis, and numerical realization of microaggregates in soils. These microaggregates have the size of a few hundred micrometers and can be understood as the fundamental building units of soil. Thus, understanding their dynamically evolving, three-dimensional structure is crucial for modeling and interpreting many soil parameters such as diffusivities and flow paths that come into play in CO$_2$-sequestration or oil recovery scenarios.

Among others, the following aspects of the formation of microaggregates should be incorporated into a mathematical model and investigated in more detail: the spatial heterogeneity of the temporally evolving structure of microaggregates and the different processes that take place on different scales — temporal and spatial — within the so-called micro-scale itself. This work aims at formulating a process-based pore-scale model, where all chemical species are measured in concentrations. That is, we have a continuous model for reactive transport mainly in terms of partial differential equations (PDEs) with algebraic constraints. This continuous model is defined on a discrete and discretely moving domain whose geometry changes according to the rules of a cellular automaton method (CAM). These rules describe the restructuring of the porous matrix, growth and decay of biomass, and the resulting topological changes of a wetting fluid and a gas phase. The cellular automaton rules additionally imply stochastic aspects that are important on the pore-scale.

Moreover, effects and knowledge deduced from the model are transferred to scales which are more relevant for applications. The quality of these averaged models is of general interest, since simulations for the field-scale that resolve the pore-scale are not applicable for economical reasons. Thus, this manuscript compares parameterizations of diffusivities with mathematically rigorous results and gives suggestions to improve the formulas that can be found in the literature.
Chapter 1 Introduction

The discrete movement of the microaggregates’ geometry at the micro-scale poses mathematical problems. The following question arises: Can the averaged quantities deduced from the pore-scale really be used for models on other scales or are the impacts of the artificial temporal jumps too detrimental for the solutions on other scales to be accurate? In the following, this problem is also dealt with, and the reliability of the obtained parameters is underlined.

Last but not least, it is imperative to apply a proper numerical method to implement the model in silico. The local discontinuous Galerkin (LDG) method seems to be suitable for this task, since it is locally mass-conservative and is stable for discontinuous data — that might, for example, originate from the discrete movement of the geometry or from the sharp boundaries between the different phases. Additionally, this method has no problems with complicated transfer conditions. These aspects are demonstrated in a mathematically rigorous way, and the method is improved upon by reducing the linear system of equations resulting from the discretization. This is a real enhancement, since it does not diminish the order of convergence but decreases the computational costs.

1.1 Objective of this work

The aim of this manuscript is to extend the existing models for biomass development [33, 35] and combine them with adapted models for solid restructuring [18] within microaggregates. The cellular automaton based model, which results from the combination of the aforementioned articles and contains rules for solid restructuring and biomass development, should be further enriched by a gas phase and a fluid phase. Moreover, a continuous model in terms of partial (and ordinary) differential equations with algebraic constraints describing reactive transport is intended to be added to the cellular automaton model and to characterize the temporal development of different chemical species. These chemical species might on the one hand influence the rules of the cellular automaton and on the other hand be influenced by the current distribution of the solid, bio, gas, and fluid phases. A corresponding model is consistently derived and formulated in this thesis. Afterwards, the main features of the model are presented using simulation scenarios, and the methods to infer characteristic macroscopic properties from the microaggregate model — describing the pore-scale — are studied and evaluated.

An additional objective of this work is to improve standard formulas for these characteristic properties. This is achieved by using homogenization theory for diffusion and comparing formulas from literature to results obtained by upscaling different kinds of pore scale geometries. In particular, random geometries and geometries resulting from our model for microaggregate formation are of interest,
since these geometries are assumed to dominate soil properties. In the context of upscaling, our approach must also be justified, since we homogenize discretely moving geometries. Consequently, we have to show — using stability and formal homogenization techniques — that a macroscopic model is indiscriminate against the discrete movement on the micro-scale.

The last focus of this thesis is improving the discontinuous Galerkin method. Particularly, the local discontinuous Galerkin method as introduced by Cockburn and Shu [124] is investigated. It is used to discretize the above model but tends to have problems with discontinuous diffusivities — occurring at the boundaries between different phases — and jump conditions that occur as transfer conditions, e.g. between the gas and the fluid phases. The scope of this thesis covers an extension of the local discontinuous Galerkin method to these cases, an improvement of this discretization technique by reducing the order of the ansatz-space for the flux unknowns, and numerical studies and analytical proofs confirming that both work out well. Beyond this, the adaption of the local discontinuous Galerkin method is transferred to its hybridized version. Moreover, this thesis formulates a discontinuous Galerkin scheme for the Nernst–Planck–Poisson equation on a periodic domain, where the Poisson equation has a right hand side which is a superposition of an \( L^2 \)-function and a \( \delta \)-distribution, and where the Nernst–Planck equation is only defined on parts of the periodic domain.

1.2 Outline of the thesis

At the beginning of Chapter 2, the importance of microaggregates for soil functions is stressed and modeling approaches and challenges are introduced. Moreover, the interplay between modeling and in vitro experiments in soil sciences is illuminated and a few problems of imaging techniques are presented. Afterwards, the different components of our model and their behavior is prescribed. The main part of this chapter is made up by illustrating numerical examples — showing the effects of different model components isolated and combined — and the numerical implementation of the model. Future prospects and a short review of the achieved results are presented at the end of the first part of the manuscript.

Chapter 3 deals with upscaling diffusion in porous media. First, we compare well-known formulas postulating a functional relation between porosity and diffusivity. Second, these formulas are compared to rigorously derived formulas for specific microstructures. Third, the numerical methods used to determine a relation between diffusivity on the one hand, and porosity, total surface area, and tortuosity on the other hand are presented.

Chapter 4 is devoted to the question of whether tensors generated from a temporally discrete micro-model can be used for a temporally continuous macro-
model. To determine if they can be used, a problem with at most countably many jumps in time is investigated at the beginning of the chapter. Although this is the relevant case in our model, it is further formally investigated if a homogenization formula for a temporally oscillating tensor can be found (similarly to the spatial homogenization theory).

An analysis of the used numerical methods can be found in Chapter 5. Here, the local discontinuous Galerkin method is applied to a partial differential equation arising in the model of Chapter 2. In this case, we consider a non-linear diffusion equation with a jump condition as prescribed by Henry’s law. Stability and convergence of the method applied to the aforementioned equation are proved and ansatz spaces of different polynomial orders are suggested to reduce computational costs without reducing the order of convergence. This is shown analytically and numerically, and the generality of the idea is shown via an application to the non-linear advection–diffusion equation, where a reduction of the computational costs without reducing the order of convergence can also be shown. And last but not least, the achieved results are transferred to a hybridized version of the scheme.

The presented manuscript is brought to a close by some concluding remarks and future research prospects in Chapter 6.

1.3 Previously published articles

Vast parts of this thesis have already been published in the form of articles. These articles are:


1.3 Previously published articles


Andreas Rupp is the main author of the articles above. The coauthors Peter Knabner, Vadym Aizinger, Jochen Schütz, Raphael Schulz, and Clint Dawson have contributed to these publications in the scope of supervision of A. Rupp. The coauthors Nadja Ray, Alexander Prechtel, and Kai Uwe Totsche held supervisory roles to [2–4, 12], respectively. The contribution of Andreas Rupp at [11] is “AR discretized and implemented the numerical model, and conducted the simulations” (cf. [11, Author Contributions]).

Section 5.3 is a result of the collaboration with Vadym Aizinger, Balthasar Reuter, and Peter Knabner. Vadym Aizinger and Peter Knabner contributed by supervision, while Andreas Rupp performed the analysis and Balthasar Reuter the implementation of the proposed method.

Section 5.4 stems form Markus Musch’s Master’s Thesis, which was supervised by Andreas Rupp. A similar version of this section has been submitted to a scientific journal and is currently being reviewed.

In addition to the already mentioned publications, Andreas Rupp is coauthor of the preprints and articles


All of these four publications will not be used in the rest of this monograph.
Chapter 2
Model for microaggregate development

Abstract of the chapter. Structure formation and self-organization in soils determine soil functions and regulate soil processes. Mathematically based modeling can facilitate the understanding of organizing mechanisms at different scales provided that the major driving forces are taken into account. However, upscaling transport in porous media including both biomass development and simultaneous structural changes in the solid matrix is extremely challenging. This is because both affect the medium’s porosity as well as the mass transport parameters and flow paths. In the following, this challenge is addressed by a multiscale model.

At the pore-scale, the local discontinuous Galerkin (LDG) method is used to solve differential equations describing the development of bacteria and of several — possibly charged — chemical species which might exist within the fluid, bio, and gas phases and on the solid boundaries. Likewise, a gluing agent tightening together solid or bio components is considered. This is combined with a cellular automaton method (CAM) capturing structural changes of the underlying computational domain stemming from biomass development, the restructuring of solid building units (which have arbitrary shapes and charges), and the reorganization of the gas phase.

Findings from standard homogenization theory are applied to determine the characteristic time- and space-dependent properties of the macroscopic medium. Investigating these results enhances our understanding of the strong interplay between the functional properties and the geometric structure of a medium. Finally, integrating such properties as model parameters into models defined on a larger scale enables representing the impact of pore-scale processes on the larger scale.

Additionally, the operational comprehensive model allows to study structure formation as a function of e.g. the size and shape of solid particles. As a process-based tool to study the interplay of relevant mechanisms in silico it represents a
Chapter 2 Model for microaggregate development

first step to capture various aspects of structure formation and self-organization in soils.

Outline of the chapter. The chapter starts with Section 2.1, where the model is motivated, and an overview over the present state of research is given. Section 2.2 introduces the model and describes its continuous and discrete parts. The used discretization methods are briefly described in Section 2.3. More details about the used methods can be found in Section 2.B and Chapter 5. Based on these numerical methods, an evaluation of the prescribed effects is conducted in Section 2.4 using simulation scenarios. A section containing conclusions and future prospects, and several appendices (including a nomenclature which also describes the respective abstract physical units of the quantities) complete the chapter.

Previously published articles. Large parts of the following chapter have already been published in


2.1 Introduction and motivation

Soils’ functions are intimately linked to their heterogeneous and dynamically evolving three-dimensional structure. Particle (dis-)aggregation under the influence of microbial activity and biofilm growth or decay within soils (or porous media in general) strongly influences their characteristic properties such as porosity
and mass transport parameters (e.g., effective diffusivity, or flow paths). Determining the evolution of such properties in space and time is demanding both at the pore-scale and at the laboratory- or field-scale. Hence, very little is known about the temporal evolution of such structures on the scale of microaggregates (typically less than 250 microns), and only recently new experimental techniques allow investigations on these scales [36]. Nevertheless, accessing three-dimensional imaging data of porous structures in combination with their inhabiting biomass at a high spatial resolution remains challenging. As a consequence, the mathematical modeling of the quantitative relationship between structure and its functional properties based on theoretical concepts is desirable across scales.

To date researchers have developed a variety of biofilm models, also formulated at different scales, ranging from continuum models and models based on cellular automaton methods (CAM) to individual based models [42]. Cooper et al. [17], e.g., used X-ray computed tomography images of natural soils to derive water retention curves with the help of mathematical homogenization from Cahn–Hilliard–Stokes equations. Similar techniques are also used in [28] to analyze the impact of roots growing through soil. Vasilyeva et al., on the other hand, provide a non-linear model that links the behavior on the micro-scale to macroscopic effects in [40]. A space-time chaos analysis of a similar model is conducted in [44]. The importance of pedotransfer functions as tools to link available soil information to properties and variables that describe soil processes is stressed in [39] and a review of approaches of such functions is given. To this end, the influence of the microstructure on wetting/drying events is analyzed in [19].

In combination with experiments, the CAM has successfully been used to describe the structural development of biofilm at the pore-scale [33, 35]. In these publications straightforward biomass spreading rules are prescribed, which allow a very flexible formulation of geometric changes, potentially also including stochastic aspects. With regard to changes in the soil’s structure, in [18] the feedback between structure and microbial activity was investigated. There, stabilizing gluing agents, which stem from biological activity and enhance the binding of soil particles, were investigated and their affinities calculated. However, the focus was placed on the self-organization of soil–microbe systems by means of stabilizing agents and not on the volume effects that are created by growing or decaying biomass. But — beyond the approaches of the aforementioned literature — particle aggregation in soils also strongly depends on the characteristic properties of the system such as particle shape or charge.

Despite the progress in describing the underlying pore-scale geometries of natural soils at a fixed time with the help of advanced imaging techniques (static approach), to my knowledge no model allows a fully dynamic and mechanistic evolution of the soil structure. An operative tool based on mechanistic principles
that allows to study *in silico* the formation of such aggregates thus could be helpful to supplement *in vitro* experiments and also provide a link to soil functions like water retention curves. The importance to study heterogeneous, evolving microstructures has also been emphasized in the context of biofilms by Brangari et al. [15], who developed a mechanistic model for biofilms in *variably saturated soils* using idealized geometries and studied the consequence on the hydraulic properties.

However, aiming to understand flow and transport in the soil at larger scales, pure pore-scale simulations are impractical due to high computational costs. To this end and to cross scales, the following research has been undertaken in the context of biofilms: In [27] and [30] a volume averaging technique was applied to an equilibrium and a non-equilibrium continuum pore-scale model for transport in biofilm and fluid with inter-phase mass transfer and biologically mediated reactions. In [31] a continuum flow model was fully coupled with a continuous biomass–nutrient growth model and the Darcy conductivity was calculated. In doing so for each time step the computational results of the flow model were upscaled using volume averaging techniques. Further upsampling methods have been applied to problems including biofilm development. However, tracking the evolving biofilm interface is in general very complex to handle. In [38] biofilm growth in a thin strip was investigated and an effective model was derived using formal two-scale asymptotic expansion in a level-set framework. The same methods were applied to a more sophisticated model in [32]. Moreover, for the resulting effective model, existence and uniqueness of weak solutions were shown. In [34] a hybrid model was developed, coupling pore-scale subdomains and continuum subdomains by means of the Mortar method. Hereby, the biofilm development was simulated at the pore-scale by means of the cellular automaton method.

In this research, several of the aforementioned processes are combined — biomass development, structural changes in the solid originating from stabilizing gluing agents, different shapes, and different charges of particles, temporal evolution of a gas phase, etc. — in a comprehensive pore-scale model. To that end, a combined discrete–continuum approach is envisaged which omits the explicit tracking of interfaces as it is necessary in level-set approaches. The movement (diffusion) of mobile bacteria, possibly transforming into immobile biomass, and other chemical species (e.g. oxygen) are prescribed by means of partial differential equations (PDEs) which are numerically solved using the local discontinuous Galerkin (LDG) method, as described in [1, 9, 10], Chapter 5, and Section 2.B. Likewise, the surface concentration of a gluing agent tightening together solid and bio cells (in the cellular automaton context) is considered. However, the underlying time-dependent computational domain, i.e. the distribution of solid, bio,
fluid, or gas cells is determined discretely by means of a cellular automaton method.

To study the formation of microaggregates from building units of different types with varying charges, shapes, and properties — like goethite, illite, or quartz as presented in [36] — prototypes of building units have been implemented to represent different geometric structures. Finally, a gas phase is incorporated into the model to account for situations where the aggregates are not fully saturated but coated only by a thin film of water, which is the wetting fluid compared to air. A restructuring of the solid phase may then induce the necessity of a reorganization of the gas phase to keep the non-wetting property. This is incorporated into the CAM rules. Exchange between and transport within the different phases may become prominent since mobility of species is highly different within the respective phases fluid, gas, or bio. If applicable, the exchange with the gas phase is implemented via Henry’s law in our model. Since electric forces are an important driving force for aggregation [36] the Nernst–Planck–Poisson equations are applied to determine the movement of ions. Furthermore, homogeneous chemical reactions (e.g. described via the mass action law) are considered within the fluid, bio and gas phases as well as heterogeneous reactions with the solid phase. The latter ones are incorporated via a kinetic rate description according to Langmuir into the model.

One main objective of this research is to examine the strong interplay between functional properties and geometric structure. To that end standard homogenization results are used to compute the soil’s characteristic properties such as porosity or effective diffusion tensors for the resulting complex and time-dependent geometries. Several scenarios are numerically evaluated in two spatial dimensions and the results are discussed thoroughly focusing on the influencing conditions for structure formation, e.g. the influence of charged building units and ions in the fluid, the influence of the range of attraction of building units, the influence of the shape of building units, and the influence of a gas phase where some dissolved species might occur — and take part at different reactions than in the fluid — and others are not present.

Another focus is to further evaluate the model’s applicability at larger scales. Consequently, a weakly coupled multiscale simulation scenario is investigated. In this setting the impact of the potentially changing yet microscopic geometry on macroscopic effects is discussed carefully.

### 2.2 Geometric setting and mathematical model

The following model has been implemented in two and three spatial dimensions. However, most of its description and the numerical experiments are done for the
two dimensional case, but they can easily be transferred to the three dimensions. The quadratic (cubic) domain \( Y \) is divided into \( N \times N \times N \) cells. We discriminate between gas cells \( Y_{g}^i \), fluid cells \( Y_{f}^j \), bio cells \( Y_{b}^k \), and solid cells \( Y_{s}^l \) representing the different phases implemented within the model, cf. Figure 2.1. The thick boundary indicates the boundary of the gas phase \( \partial Y_{g} \), while the double-lined boundary is the boundary of the solid phase \( \partial Y_{s} \). Note that Section 2.2.3 — describing the restructuring of the gas cells — says that \( \partial Y_{s} \) and \( \partial Y_{g} \) are very unlikely to intersect, since gas is the non-wetting phase compared to fluid. Moreover, a so called gluing agent is allowed to live on bio–bio, bio–solid, bio–fluid, bio–gas, solid–solid, solid–fluid, and solid–gas interfaces but not on interfaces between two gas, two fluid, or a fluid and a gas cell, respectively. \( \Box \) indicates a larger building unit and should be interpreted as a single larger solid block \( Y_{s}^m \). The dashed lines indicate the boundary of our periodic domain \( Y \). An overview of the behavior of the different model components is given in Table 2.2 on page 74 of this manuscript.

The model includes a combination of discrete and continuum parts: A cellular automaton method (CAM) is used to capture geometric and structural changes. The cellular automaton acts on a quadratic (cubic) domain \( Y \) with periodic bound-
2.2 Geometric setting and mathematical model

Figure 2.2: Possible shapes of building units (size not to scale); from left to right: Spherical, platy, or needle-like, and composites. Black and white indicate equal charge for the composites.

ary $\partial Y$ being covered by a regular grid containing $N^2 (N^3)$ quadratic (cubic) cells $Y^i$ with faces $\partial Y^i$. At first, one of the following cell states is assigned to each of the cells: “bio” (b), “fluid” (f), “solid” (s), or “gas” (g), cf. Figure 2.1. Note that this is distinct from real world situations, where the fluid distribution depends for instance on wettability and pore sizes. However, I want to emphasize the self-organization of the system due to the underlying mechanisms without relying on specific spatial structures. The additional consideration of more realistic structures, e.g. as a result of CT images, is focus of forthcoming research.

The cells $Y^i$ in the cellular automaton correspond to the smallest physical units in the model. Different inseparable building units with various shapes may be defined — composed of these smallest unit cells $Y^i$. We thus can consider for instance spherical geometries, needle shapes, or plates, and investigate the resulting structures. They may represent prototypes of, e.g., quartz, goethite, or illite particles, cf. Figure 2.2 or $\mathcal{A}$ in Figure 2.1. Additionally, composites of different building units may be considered, cf. Figure 2.2.

The union $\bigcup_i Y^i_s$ of all solid cells is termed the solid phase and denoted by $Y_s$ with boundary $\Gamma := \partial Y_s$. Likewise, the union $\bigcup_i Y^i_b$ of all bio cells — the bio phase — is denoted by $Y_b$, the union $\bigcup_i Y^i_f$ of all fluid cells — the fluid phase — by $Y_f$, and the union $\bigcup_i Y^i_g$ of all gas cells — the gas phase — by $Y_g$, cf. Figure 2.1. Furthermore, we denote the union of fluid and bio phases with the liquid phase and define the interface $\Gamma_{LG} := (\partial (Y_f \cup Y_b)) \cap \partial Y_g$ of the gas with the liquid phases. In each time step a redistribution of the respective phases is defined according to restructuring / growing and shrinking / reorganizing rules in the cellular automaton framework, cf. [3] and Section 2.2.3.

Within the fluid, bio, and gas phases, the continuum parts of the model come into play. Here, (possibly coupled, partial) differential equations are solved for the transported, potentially charged chemical species, and also the immobile biomass. Likewise, an ordinary differential equation is considered for the gluing agent (e.g. extracellular polymeric substances (EPS)), possibly being present on $\bigcup_i \partial Y^i_s \cup \bigcup_i \partial Y^i_b$ and holding together bio and/or solid cells.
2.2.1 Model parts

Within the model, we essentially consider the following prototypical time- and space-dependent model parts:

1. A **solid phase** (s). *Gluing agent* (α) may be present on the solid surfaces, and also (variable) **surface charges** which influence the restructuring rules among solid building units. Additionally, heterogeneous reactions with mobile chemical species may take place on the solid surfaces.

2. A **fluid phase** (f), the **wetting phase** (e.g., water) containing **mobile and reacting, potentially charged chemical species**, i.e.
   - several types of mobile ions/molecules potentially participating at heterogeneous or homogeneous reactions,
   - one prototype of diffusing nutrient, for example oxygen (note that oxygen is a molecule but since it is the nutrient for bacteria it is treated differently than the other molecules/ions),
   - and several types of diffusing bacteria (Bac) consuming oxygen.

3. A **bio phase** (b) in which the above species diffuse with lower **diffusivity** and **mobility** than in the fluid. Moreover, **biomass** is created if the bacteria exceed a certain predefined threshold in the fluid. It decays and grows depending on the availability of nutrient and bacteria in the bio cells, and gluing agent may further influence the attachment of particles (see Section 2.2.2).

4. **Gas** (g) — the **non-wetting phase** — where some of the above species diffuse with the highest diffusivity. Since fluid is supposed to be the wetting fluid, the gas phase is supposed to have as few common interfaces with the solid phase as possible. For that reason, gas cells reorganize whenever solid cells have moved and become neighbors of gas cells. Some species are supposed to live within fluid, bio, and gas cells. For these species *Henry’s law* is supposed to hold on \( \Gamma_{LG} = (\partial(Y_f \cup Y_b)) \cap \partial Y_g \). The remaining species are supposed to live only in \( Y_f \cup Y_b \) and the gas phase limits their movement.

Finally, the nutrient is consumed by biomass, bacteria, and gluing agent. Remember that the gluing agent is possibly present at the solid cells’ interfaces (i.e. solid–solid, solid–bio, solid–fluid, and solid–gas interfaces) and bio cells’ interfaces (i.e. bio–bio, bio–fluid, bio–solid, and bio–gas interfaces), but not at the fluid–fluid, fluid–gas, or gas–gas cells’ interfaces. Following [18] we assume that the (stabilizing) **gluing agent** (e.g. EPS) is produced as a consequence of local biotic activity at the solid blocks’ boundaries and assume its production to be proportional to the local **respiration rate** while its relative decay rate is constant. The biomass can be interpreted as agglutinated bacteria.

The model parts and their specific features are clearly arranged recapitulated in Table 2.2 on page 74.
2.2 Geometric setting and mathematical model

2.2.2 Continuum model parts

Within the continuum part of the model, differential equations are solved for the diffusing species, the gluing agent, and the biomass. More precisely, the Nernst–Planck equation with additional reaction terms is solved for ions and molecules (for which it simplifies to a system of diffusion–reaction equations). Diffusion–reaction equations are also formulated for the transport of the nutrient concentration \( c_{O_2} \) and the bacteria concentration \( c_{Bac} \) (although they are a special case of the more general equations). Here, it must be recognized that the differential equations are defined in the time-dependent domain \( Y_f \cup Y_b \cup Y_g \) (or \( Y_f \cup Y_b \) for species which do not exist in the gas phase). The details about the set of equations can be found in the following, where the binary operator “\( \ominus \) — due to the time-dependence of the domain \( \times \) cannot be used — is defined by

\[
(0, T) \ominus \Omega(t) := \bigcup_{t \in (0, T)} \{t\} \times \Omega(t).
\]

Equations for nutrient, bacteria, biomass, and sticky agent. The molecular diffusivities for the nutrient are denoted by \( D_{O_2,b}, D_{O_2,f}, \) and \( D_{O_2,g} \) within the bio, the fluid, and the gas cells, and for the bacteria by \( D_{Bac,b} \) and \( D_{Bac,f} \), respectively. Note that both diffusivities \( D_{O_2} \) and \( D_{Bac} \) are discontinuous since they differ within different phases, \( \Gamma_{LG} = (\partial(Y_f \cup Y_b)) \cap \partial Y_g \), \( \nu \) is the unit outward normal with respect to \( Y_f \cup Y_b \) or \( Y_f \cup Y_b \cup Y_g \), respectively, and \( \nu_g \) is the unit outward normal with respect to \( Y_g \).

\[
\begin{align*}
\partial_t c_{O_2} - \nabla \cdot \left( D_{O_2,b/f/g} \nabla c_{O_2} \right) &= R_{O_2} \quad \text{in} \ (0, T) \ominus (Y \setminus Y_s) \quad (2.1a) \\
\left(-D_{O_2,b/f/g} \nabla c_{O_2}\right) \cdot \nu &= 0 \quad \text{on} \ (0, T) \ominus \partial Y_s \quad (2.1b) \\
c_{O_2,b/f} / c_{O_2,g} = H_{O_2}^{\Gamma_{LG}} \quad \text{on} \ (0, T) \ominus \Gamma_{LG} \quad (2.1c) \\
(D_{O_2,g} \nabla c_{O_2})|_{Y_g} \cdot \nu_g - (D_{O_2,b/f} \nabla c_{O_2})|_{Y_f \cup Y_b} \cdot \nu_g &= 0 \quad \text{on} \ (0, T) \ominus \Gamma_{LG} \quad (2.1d)
\end{align*}
\]

\[
\begin{align*}
\partial_t c_{Bac} - \nabla \cdot \left( D_{Bac,b/f} \nabla c_{Bac} \right) &= R_{Bac} \quad \text{in} \ (0, T) \ominus (Y_f \cup Y_b) \quad (2.2a) \\
\left(-D_{Bac,b/f} \nabla c_{Bac}\right) \cdot \nu &= 0 \quad \text{on} \ (0, T) \ominus \partial (Y_f \cup Y_b) \quad (2.2b)
\end{align*}
\]

(2.1c) and (2.1d) implement Henry’s law for oxygen describing the phase transition between the aqueous and the gas states of oxygen at thermodynamical equilibrium under low pressure gradients, and for low concentrations of ions. Here, \( H_{O_2}^{\Gamma_{LG}} \) is the Henry’s law solubility constant for oxygen and describes the ratio of the concentrations of oxygen in the liquid (bio and fluid) and the gas phases.
(2.2a) describes the diffusion of bacteria within the fluid and bio cells, where their movement is restricted. Thus, \( D_{\text{Bac,b}} \) is much smaller than \( D_{\text{Bac,f}} - D_{\text{Bac,b}} \) could even be zero indicating that bacteria are immobile within the bio phase, but is assumed to be a small positive number in the rest of this thesis. (2.2b) specifies a zero flux boundary at solid and gas boundaries, although some bacteria do adsorb onto solid surfaces [37] or accumulate at the gas–liquid interface in porous media [41]. This clearly should be taken into account in future research, but is disregarded in the following.

Note that the domain \( Y \) is periodic which, in particular, implies periodic boundary conditions for the nutrient and bacteria on \( \partial Y \). Moreover, appropriate initial conditions are prescribed to close the problem. For each simulation scenario, they will be specified.

In the following, we discuss the transformation of bacteria into biomass, its growth and decay, the evolution of the gluing agent’s concentration, and the consumption of the nutrient which is inherent to both processes. In this sense, internal sources or sinks are included in the model equations (2.1) and (2.2). More precisely, the nutrient sinks which are related to its consumption by the gluing agent, bacteria, and biomass, and the transformation of the bacteria into biomass, i.e. a sink for bacteria, are discussed below.

First, the transformation of a fluid cell into a bio cell is accompanied with the generation of biomass from bacteria, its growth, and its decay. The transformation of a fluid cell \( Y^i_f \) into a bio cell \( Y^i_b \) occurs if the bacteria exceed a certain threshold \( \int_{Y^i_f} c_{\text{Bac,max}} \, dx \) in the respective cell, i.e. if

\[
\int_{Y^i_f} c_{\text{Bac}} \, dx > \int_{Y^i_f} c_{\text{Bac,max}} \, dx.
\]

Then, the bacteria completely transform into biomass and their concentration \( c_{\text{Bac}} \) becomes zero in this cell, cf. (2.3b). Simultaneously, the biomass concentration \( c_B \) takes a constant value within the newly created biomass cell \( Y^i_b \leftarrow Y^i_f \) as defined in (2.3a). Note that, on the contrary, bio cells turn into fluid cells if the biomass concentration reaches the minimum biomass concentration \( c_{B,\text{min}} \).

\[
c_B = \frac{1}{|Y^i_b|} \int_{Y^i_b} c_{\text{Bac}} \, dx \quad \text{in } Y^i_b, \quad \tag{2.3a}
\]

\[
c_{\text{Bac}} = 0 \quad \text{in } Y^i_b. \quad \tag{2.3b}
\]

Within the bio phase \( Y_b \) a generation of biomass from bacteria takes place. Moreover, biomass and bacteria growth by means of the nutrient takes place in \( Y_b \), and in the bio and the fluid cells \( Y_b \cup Y_f \) (cf. Equation 2.2a), respectively.

\[
\partial_t c_B = f_{\text{growth/decay,B}}(c_B, c_{O_2}) + f_{\text{increase,B}}(c_{\text{Bac}}, c_B) \quad \text{in } (0, T) \otimes Y_b,
\]
2.2 Geometric setting and mathematical model

\[ R_{Bac} = f_{growth,Bac}(c_{O_2}) + f_{decay,Bac}(c_{Bac}) + f_{decrease,Bac}(c_{Bac}, c_B) \text{ in } (0, T) \otimes (Y_f \cup Y_b). \]

The implementation of different rates into the model is straightforward. The used ones are defined as follows: For the biomass growth and decay \( f_{growth/decay} \), we assume a dependence on the availability of nutrient in the respective cell \( Y_i^{t} \). That is, biomass grows if the average nutrient concentration is larger than the constant \( c_{up,O_2,min,B} \) and decays otherwise. More precisely, a linear rate (first order kinetics) is chosen for the decay of biomass and a constant rate (zeroth order kinetics) is chosen for the growth of biomass.

The increase \( f_{increase,B} \) in the biomass depends on the availability of bacteria diffusing in the bio cell. Assuming that the consumption of bacteria by biomass, which actually is a transformation of bacteria into biomass, depends linearly on the concentration of bacteria and linearly on the concentration of biomass \( c_B \), between 20% (when \( c_B = c_{B,min} \), the prescribed minimum amount of biomass within a cell) and 80% (when \( c_B = c_{B,max} \), the prescribed maximum amount of biomass in a cell) of the available bacteria are consumed. At the same time, the bacteria concentration \( c_{Bac} \) decreases at the same rate. The constants 20% and 80% are chosen exemplarily here. Finally, a linear rate (first order kinetics) is given for the decay of bacteria and a constant rate (zeroth order kinetics) is chosen for the growth of bacteria depending on the availability of the nutrient. This yields similar rates for biomass and for bacteria:

\[
(f_{growth/decay,B})(c_B, c_{O_2}) = \begin{cases} 
-k_{d,B}c_{Bac}, & \text{if } \int_{Y_b} c_{O_2} \, dx \leq \int_{Y_b} c_{up,O_2,min,B} \, dx, \\
\text{const}_1, & \text{if } \int_{Y_b} c_{O_2} \, dx > \int_{Y_b} c_{up,O_2,min,B} \, dx 
\end{cases} \text{ in } (0, T) \otimes Y_b^{t},
\]

\[
f_{increase,B}(c_{Bac}, c_B) = \frac{0.6c_B + 0.2c_{B,max} - 0.8c_{B,min}}{c_{B,max} - c_{B,min}} c_{Bac} \text{ in } (0, T) \otimes Y_b,
\]

\[
f_{growth,Bac}(c_{O_2}) = \begin{cases} 
0, & \text{if } c_{O_2} \leq 0, \\
\text{const}_2, & \text{if } c_{O_2} > 0 
\end{cases} \text{ in } (0, T) \otimes (Y_b \cup Y_f),
\]

\[
f_{decay,Bac}(c_{Bac}) = -k_{d,B}c_{Bac} \text{ in } (0, T) \otimes (Y_b \cup Y_f),
\]

\[
f_{decrease,Bac}(c_{Bac}, c_B) = -f_{increase,B}(c_{Bac}, c_B) \text{ in } (0, T) \otimes Y_b.
\]

Finally, following the ideas and using similar rates as in [18], the concentration \( c_a = (c_{a,ik})_{i,k \in \{1, \ldots, N^2\}} \) of the gluing agent (called activity in [18]) is defined, which is actually a surface concentration. Of course, other rate formulations can easily be plugged in the equation system. Since there is no agent present at the fluid–fluid, fluid–gas, and gas–gas interfaces, for each time step the support is at most \( \cup_j \partial Y_i^{t} \cup \cup_j \partial Y_i^{t} \), i.e. all solid–solid, solid–bio, solid–fluid, solid–gas, bio–fluid, bio–gas, and bio–bio interfaces. The concentration of the gluing agent
is time-dependent, but section-wise constant in space, i.e. constant along the single cell faces $\partial Y^k \cap \partial Y^l$. It is prescribed via

$$
\partial_t c_\alpha = \begin{cases} 
 f_{\text{increase}, \alpha}(c_{O_2}) + f_{\text{decay}, \alpha}(c_\alpha) & \text{on } (0, T) \otimes \left( \bigcup_i \partial Y^i_s \cup \bigcup_i \partial Y^i_b \right), \\
 0 & \text{else.}
\end{cases} \tag{2.4}
$$

Following the same practice as in [18], in our simulations the reaction rates are defined as follows: For the decay we assume first order kinetics. For an increase in the gluing agent’s concentration, we assume a dependence on the availability of nutrient, i.e. the rate is zero if no nutrient is available or a zeroth order kinetics if nutrient is available in the neighboring cells, respectively. However, since gluing agent is related to biomass extracellular polysaccharides a considerable alternative to the above formulation is to allow an increase of gluing agent only to happen on biomass faces. The resulting equation (2.18) can be found on page 74. For its evaluation, note that according to (2.1), there is no nutrient present in any solid cell $Y^i_s$, that $c_{\up, O_2, \min, \alpha}$ is a given constant, and that the components $(f_{\text{increase}, \alpha})_{lk}$ of the rate may only be non-zero for non fluid–fluid, non fluid–gas, or non gas–gas interfaces, i.e. $(Y^l \not\subset Y_f \cup Y_g)$ or $(Y^k \not\subset Y_f \cup Y_g)$ cf. (2.4).

$$
f_{\text{decay}, \alpha}(c_\alpha) = -k_{d, \alpha} c_\alpha \quad \text{on } (0, T) \otimes \left( \bigcup_i \partial Y^i_s \cup \bigcup_i \partial Y^i_b \right). \tag{2.4}
$$

Since biomass, bacteria, and also gluing agent consume nutrient, the nutrient’s right hand side looks as follows:

$$R_{O_2} = -f_{\up, O_2, \alpha}(c_{O_2}) - f_{\up, O_2, B}(c_{O_2}) - f_{\up, O_2, Bac}(c_{O_2}),$$

with

\begin{align*}
(f_{\up, O_2, \alpha})_k(c_{O_2}) &= \begin{cases} 
0, & \text{if } \int_{Y^k} c_{O_2} \ dx \leq \int_{Y^k} c_{\up, O_2, \min, \alpha} \ dx, \\
\text{const}_k, & \text{if } \int_{Y^k} c_{O_2} \ dx > \int_{Y^k} c_{\up, O_2, \min, \alpha} \ dx
\end{cases} \quad \text{in } Y^k, \\
(f_{\up, O_2, \alpha})_l(c_{O_2}) &= \begin{cases} 
0, & \text{if } \int_{Y^l} c_{O_2} \ dx \leq \int_{Y^l} c_{\up, O_2, \min, \alpha} \ dx, \\
\text{const}_l, & \text{if } \int_{Y^l} c_{O_2} \ dx > \int_{Y^l} c_{\up, O_2, \min, \alpha} \ dx
\end{cases} \quad \text{in } Y^l, \\
(f_{\up, O_2, B})_i(c_{O_2}) &= \begin{cases} 
0, & \text{if } \int_{Y^i_b} c_{O_2} \ dx \leq \int_{Y^i_b} c_{\up, O_2, \min, B} \ dx, \\
\text{const}_b, & \text{if } \int_{Y^i_b} c_{O_2} \ dx > \int_{Y^i_b} c_{\up, O_2, \min, B} \ dx
\end{cases} \quad \text{in } Y^i_b, \\
f_{\up, O_2, Bac}(c_{O_2}) &= \begin{cases} 
0, & \text{if } c_{O_2} \leq 0, \\
\text{const}, & \text{if } c_{O_2} > 0
\end{cases} \quad \text{in } (0, T) \otimes (Y_b \cup Y_f). \end{align*}
Furthermore, note that the agent is a \textit{surface-related} quantity and the nutrient concentration is a \textit{volume-related} quantity. Consequently, the respective quantities “\textit{const}” in the rates for the agent must be scaled with a factor. The gluing agent glues together discrete solid or bio cells and consequently finally contributes to the change of the solid/bio structure, see Section 2.2.3 for the corresponding restructuring rules.

**Equations for molecules and ions.** In the following, we consider the concentrations of the charged species $\omega_{r}^{\pm}$ (with discontinuous \textit{diffusivity} $D_{r}$, electric \textit{drift constant} $C_{r}$, and the superscript indicating positive or negative charge) in the fluid, and $\omega_{r}^{F,\pm}$ on the solid phase’s boundary $\Gamma := \partial Y_s$. The following set of equations is supposed to be satisfied:

\begin{align}
\partial_t \omega_{r}^{\pm} \pm \nabla \cdot (C_{r} \omega_{r}^{\pm} E) - \nabla \cdot (D_{r} \nabla \omega_{r}^{\pm}) &= R_{r}(\omega) \quad \text{in} \quad (0, T) \cap (Y_f \cup Y_b), \quad (2.5a) \\
G_{r}(\omega, \partial_t \omega, \omega_{r}^{F}) - \partial_t \omega_{r}^{F} &= 0 \quad \text{on} \quad (0, T) \cap \Gamma, \quad (2.5b) \\
\pm (C_{r} \omega_{r}^{\pm} E) \cdot \mathbf{v} - (D_{r} \nabla \omega_{r}^{\pm}) \cdot \mathbf{v} &= 0 \quad \text{on} \quad (0, T) \cap \Gamma_{LG}, \quad (2.5c) \\
\omega_{r}^{\pm} &= \omega_{r,0} \quad \text{in} \quad \{0\} \cap (Y_f \cup Y_b), \quad (2.5d)
\end{align}

that is, ions are supposed to be transported in terms of an \textit{advection–diffusion–reaction equation} where the advective flux can be interpreted as proportional to the \textit{electric field} $E$. The \textit{homogeneous reactions} are represented by their reaction rate $R_{r}$, the \textit{heterogeneous reactions} are described by $G_{r}$, and $\omega (\omega_{r}^{F})$ is a vector containing the concentrations of all species — charged and uncharged — in the fluid (on the solid phase’s boundary).

We want to find appropriate closing (conservative boundary) conditions for (2.5). Thus, having integrated over the time-dependent domain $Y_f \cup Y_b =: \bar{Y}(t)$ we expect (for a continuous model and due to physical correctness) that the \textit{continuity equation}

$$
\frac{d}{dt} \left[ \int_{\bar{Y}(t)} \omega_{r}^{\pm} \, dx + \int_{\partial \bar{Y}(t)} \omega_{r}^{F,\pm} \, d\sigma \right] = \int_{\bar{Y}(t)} R_{r}(\omega) \, dx
$$

holds. This needs that $\bar{Y}(t)$ moves continuously. However, our model can be interpreted as discrete version of this continuous setting. Having defined $X(t; x_0)$ as the so-called \textit{trajectory} or \textit{flight path} of a molecule/ion that is located at the spatial point $x_0$ and the time $t_0$, $J(t; x)$ as its (spatial) \textit{Jacobian determinant}, $v(t, X(t, x)) := \partial_t X(t, x)$ as its \textit{velocity}, and neglecting the subscript $r$ and superscript $\pm$ we can deduce that

$$
\frac{d}{dt} \int_{\bar{Y}(t)} \omega(t, x) \, dx = \frac{d}{dt} \int_{\bar{Y}(0)} \omega(t, X(t; x)) \, J(t; x) \, dx
$$
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\[
\begin{align*}
&= \int_{\mathcal{Y}(t)} \left[ \left( \frac{\partial}{\partial t} \omega(t, X(t; x)) \right) J(t; x) + \omega(t, X(t; x)) \left( \frac{\partial}{\partial t} J(t; x) \right) \right] \, dx \\
&= \int_{\mathcal{Y}(t)} \left[ \partial_t \omega(t, X(t; x)) + \nabla \omega(t, X(t; x)) \cdot \partial_t X(t; x) \\
&\quad \quad + \omega(t, X(t; x)) (\nabla \cdot \partial_t X(t; x)) \right] J(t; x) \, dx \\
&= \int_{\mathcal{Y}(t)} \partial_t \omega(t, x) \, dx + \int_{\mathcal{Y}(t)} \nabla_x \cdot (\omega(t, x) \nu(t, x)) \, dx \\
&= \int_{\mathcal{Y}(t)} \partial_t \omega(t, x) \, dx + \int_{\partial \mathcal{Y}(t)} (\omega(t, x) \nu(t, x)) \cdot \nu \, d\sigma
\end{align*}
\]

if we assume all terms to be sufficiently regular. Assuming that \( \|\nu\| \) is small — since our domain moves quite slowly (i.e. in the range of \( \mu m \) per day) — we receive

\[
\frac{d}{dt} \int_{\mathcal{Y}(t)} \omega(t, x) \, dx \approx \int_{\mathcal{Y}(t)} \partial_t \omega(t, x) \, dx = \int_{\mathcal{Y}(t)} R_t(\omega) \cdot \nabla \cdot (C \cdot \omega^{\xi} E) + \nabla \cdot (D \cdot \omega^{\xi}) \, dx.
\]

To gain a similar result for the boundary concentration \( \omega^f \) we define \( A : \mathbb{R}^{n-1} \supset M \rightarrow \partial \mathcal{Y}(0) \subset \mathbb{R}^n, \Phi : [0, T] \times M \rightarrow \partial \mathcal{Y}(t) \) by \( \Phi(t, \xi) = X(t; A(\xi)) \), and \( \phi := \sqrt{\det D_\xi \Phi^T D_\xi \Phi} \). Implying the assumption that the boundary can be described by a single mapping and does not change its topology, this yields

\[
\partial_t \phi = \frac{\phi^2}{2\phi} \text{tr} \left[ (D_\xi \Phi^T D_\xi \Phi)^{-1} \partial_t (D_\xi \Phi^T D_\xi \Phi) \right] = \phi \text{tr} \left[ \left( D_\xi \Phi^T D_\xi \Phi \right)^{-1} D_\xi \Phi^T \partial_t D_\xi \Phi \right] = D_\xi \Phi^+ \partial_t D_\xi \Phi
\]

and allows for the following equations

\[
\begin{align*}
\frac{d}{dt} \int_{\partial \mathcal{Y}(t)} \omega^f(t, x) \, d\sigma &= \frac{d}{dt} \int_M \omega^f(t, \Phi(t, \xi)) \phi \, d\xi \\
&= \int_M \left[ \partial_t \omega^f(t, \Phi(t, \xi)) + \nabla \omega^f(t, \Phi(t, \xi)) \cdot \partial_t \Phi(t, \xi) \right] \phi(t, \xi) \, d\xi \\
&\quad + \int_M \omega^f(t, \Phi(t, \xi)) \partial_t \phi(t, \xi) \, d\xi \\
&= \int_{\partial \mathcal{Y}(t)} \left[ \partial_t \omega^f(t, x) + \nabla_x \omega^f(t, x) \cdot \nu(t, x) \right] \, d\sigma \\
&\quad + \int_M \left[ \omega^f(t, \Phi(t, \xi)) \text{tr} \left( D_\xi \Phi^+ \partial_t D_\xi \Phi \right) \right] \phi(t, \xi) \, d\xi,
\end{align*}
\]
where $\nabla_x \omega^F$ has to be interpreted in an appropriate way (since $\omega^F$ is a boundary concentration) and $\partial_t \phi$ can be interpreted as measure for the elongation/shrinkage of the boundary (with respect to time). Thus, assuming that $|\nabla_x \omega^F \cdot v|$ is small — since our domain moves quite slowly (i.e. in the range of $\mu$m per day) and the differences in boundary concentrations are mild — and that the size (Hausdorff measure) of the boundary remains (locally) constant — i.e. not even parts of the boundary elongate or shrink with respect to time — we can deduce that

$$\frac{d}{dt} \int_{\partial Y(t)} \omega^{F,\pm}_r(t, x) \, d\sigma \approx \int_{\partial Y(t)} \partial_t \omega^{F,\pm}_r(t, x) \, d\sigma.$$  

**Remark 2.2.1.**

1. The above arguments for boundary integrals also work if the boundary cannot be described by a single mapping $\Phi$. Thus, for non-deformable building units $\tilde{Y}_i(t)$ moving through $Y$ such that $\partial \tilde{Y}_i(t) = \bigcup_i \partial \tilde{Y}_i(t)$ and with a constant concentration of $\omega^{F,\pm}_r$ on each building unit’s boundary, we have

$$\frac{d}{dt} \int_{\partial \tilde{Y}_i(t)} \omega^{F,\pm}_r(t, x) \, d\sigma = \frac{d}{dt} \int_{\partial Y_i(t)} \omega^{F,\pm}_r(t) \, d\sigma = \int_{\partial \tilde{Y}_i(t)} \partial_t \omega^{F,\pm}_r(t, x) \, d\sigma \approx \int_{\partial Y_i(t)} \partial_t \omega^{F,\pm}_r(t, x) \, d\sigma$$

i.e. the above approximative equation becomes sharp. This can also be interpreted in the way that for such building units the surfaces do not change ($\partial_t \phi = 0$) and that $\nabla_x \omega^{F,\pm}_r(t, x) = 0$ on each building unit.

2. A proof for the transport theorem on evolving hyper-surfaces which is formally described by (2.6) and more rigorously formulated as

$$\frac{d}{dt} \int_{\partial \tilde{Y}(t)} \omega^F(t, x) \, d\sigma = \int_{\partial \tilde{Y}(t)} \left( D^* \omega^F(t, x) + \omega^F(t, x) \nabla_{\partial \tilde{Y}(t)} \cdot v(t, x) \right) \, d\sigma,$$

where $D^*$ denotes the material derivative and $\nabla_{\partial \tilde{Y}(t)} \cdot v$ denotes the surface divergence of $v$ can be found in [16, Sect. 5.2] or [21].

Having plugged this into the continuity equation we receive

$$\int_{\partial \tilde{Y}(t)} \partial_t \omega^{F,\pm}_r(t, x) \, d\sigma \mp (C_r \omega^F E) \cdot v + (D_r \nabla \omega^F E) \cdot v \, d\sigma \approx 0,$$

motivating the following conservative, auxiliary boundary conditions:

$$\pm (C_r \omega^F E) \cdot v - (D_r \nabla \omega^F E) \cdot v = \partial_t \omega^{F,\pm}_r \quad \text{on} \quad (0, T) \otimes \Gamma.$$  

(2.7a)
Assuming that the domain moves quite slowly (in the range of μm per day) compared to the speed of diffusion and reactions we neglect the terms containing \(a'(t)\) or \(b'(t)\) and recognize that we have recovered the motivation for the boundary conditions that have been deduced above in a more general case i.e.

\[
\pm (C_r \omega_t^\pm E) \cdot \nu - (D_r \nabla \omega_r^\pm) \cdot \nu = \partial_t \omega_r^{G, \pm} \quad \text{on} \quad (0, T) \cap \Gamma_{LG}.
\]
2.2 Geometric setting and mathematical model

\[ \pm (C_r \omega^\pm_r E) \cdot \nu - (D_r \nabla \omega^\pm_r) \cdot \nu = 0 \quad \text{on} \quad (0, T) \otimes \Gamma_{LG}. \]

Note that assuming that \( \omega^\pm_{r,a}(t) = \omega^\pm_r(t, a(t)) \) we receive

\[ \frac{d}{dt} \omega^\pm_{r,a}(t, a(t)) = \partial_t \omega^\pm_r(t, a(t)) + \partial_x \omega^\pm_r(t, a(t)) a'(t), \]

but the terms \( \partial_t \omega^\pm_r(t, a(t)) \) and \( \partial_x \omega^\pm_r(t, b(t)) \) do not make sense in the common sense, since \( \omega^\pm_r \) is only defined on the two boundary points of the interval — a similar problem accounts for \( \nabla \omega^\pm \). In this case the normal derivative of \( \omega^\pm_r(t, a(t)) \) with respect to the boundary is supposed to be 0 since \( \frac{d}{dt} \omega^\pm_{r,a}(t) = \frac{d}{dt} \omega^\pm_{r,a}(t, a(t)) \).

The equations (2.5) and (2.7) give rise to the Nernst–Planck equations used in our model. A detailed mathematic description can be found below.

**The Nernst–Planck–Poisson equation for ions.** According to the above calculations the Nernst–Planck (NP) equations can be written in the following general form:

\[
\begin{aligned}
\partial_t \omega^\pm_r &\pm \nabla \cdot (C_r \omega^\pm_r E) - \nabla \cdot (D_r \nabla \omega^\pm_r) = R_r(\omega) \quad \text{in} \quad (0, T) \otimes (Y_f \cup Y_b), \\
G_r(\omega, \partial_t \omega, \omega^\Gamma_r, \partial_t \omega^\Gamma_r) &= 0 \quad \text{on} \quad (0, T) \otimes \Gamma, \\
\pm (C_r \omega^\pm_r E) \cdot \nu - (D_r \nabla \omega^\pm_r) \cdot \nu &= \partial_t \omega^\pm_r \quad \text{on} \quad (0, T) \otimes \Gamma, \\
\pm (C_r \omega^\pm_r E) \cdot \nu - (D_r \nabla \omega^\pm_r) \cdot \nu &= 0 \quad \text{on} \quad (0, T) \otimes \Gamma_{LG}, \\
\omega^\pm_r &= \omega^\pm_{r,0} \quad \text{in} \quad \{0\} \otimes (Y_f \cup Y_b).
\end{aligned}
\]

(2.8)

Here, the boundary conditions are chosen to be a kinetic version of those from [26, (1.6),(1.8)] — equilibrium rates would lead to contradictions (since the domain and its boundary move discretely in our model), that is

\[ G_r(\omega, \partial_t \omega, \omega^\Gamma_r, \partial_t \omega^\Gamma_r) = \partial_t \omega^\pm_r - k g(\omega^\pm_r) + k \omega^\pm_r, \]

where \( g(\cdot) \) plays the role of an equilibrium isotherm and \( k \) is a rate constant. For our model, we choose \( g \) to represent the Langmuir isotherm. Thus, \( G \) represents a kinetic reaction based on the Langmuir isotherm. Moreover, we can — according to [14, p. 1909] — write \( R_r \) in terms of the mass action law, but — for simplicity — we replace the electrochemical potentials by the concentrations of the respective species. The electric field \( E \) and electric potential \( \Phi \) are computed in terms of a Poisson equation [23, p. 45]

\[
\begin{aligned}
- \nabla \cdot (\varepsilon_r \nabla \Phi) &= \rho_e \quad \text{in} \quad (0, T) \otimes (Y_f \cup Y_b), \\
E &= - \varepsilon_0 \nabla \Phi \quad \text{in} \quad (0, T) \otimes (Y_f \cup Y_b), \\
- E \cdot \nu &= \rho_e^f \quad \text{on} \quad (0, T) \otimes \Gamma, \\
- E \cdot \nu &= 0 \quad \text{on} \quad (0, T) \otimes \Gamma_{LG},
\end{aligned}
\]

(2.9)
where \( \rho_e = \sum_{r=1}^{N} z_r \omega_r^e \) and \( \rho_e^r = \sum_{r=1}^{N} z_r \omega_r^{e,r} \) denote the total charge densities in the fluid and on the boundary, respectively. Here \( z_r \) is the charge of the \( r \)-th species and \( \epsilon_0 \) is the (discontinuous, since phase depending) dielectric permittivity.

Since (2.9) does not have a unique solution, we further need to claim that \( \forall t \in (0, T) \)

\[
\int_{Y_f \cup Y_b} \Phi \, dx = 0,
\]

and as we have

\[
\int_{Y_f \cup Y_b} \rho_e \, dx = \int_{Y_f \cup Y_b} - \nabla \cdot (\epsilon_0 \nabla \Phi) \, dx = \int_{\Gamma \cup \Gamma_G} E \cdot \nu \, d\sigma = - \int_{\Gamma} \rho_{e}^r \, d\sigma,
\]

(2.10) imposes some consistency conditions on (2.8). These consistency conditions have to ensure that the total charge density of the (whole) fluid equals the total charge density of the (whole) boundary (with a changed sign), i.e. the whole domain (including its boundary) is electrically neutral. Hence, \( R_r \) cannot be chosen randomly but has to ensure some sort of conservation of charge, while \( G \) can be an arbitrary boundary reaction, as the flux-boundary condition in (2.8) ensures conservation independently of \( G \). Moreover, the initial condition of (2.8) has to ensure (2.10).

(2.8) and (2.9) \((\omega_r^e \) and \( E)\) are coupled in a non-linear way. This coupled system of Nernst–Planck and Poisson equations is called Nernst–Planck–Poisson (NPP) equation.

In our model, the domain \( Y_s \) is allowed to change with respect to time. That is why, there could be ions between two solid building units which do not directly influence \( Y_f \cup Y_b \) or \( \Gamma \). This contradicts (2.10) and does not allow a solution of (2.9) to exist. To solve this problem, we extend the electric field onto our whole domain \( Y \) and reinterpret the ions on the boundaries of solid building units \( \Gamma_s = \bigcup_{i} \partial Y_i^s \) as sub-dimensional sources or sinks of our electric potential \( \Phi \). It is important to note that the dielectric permittivity \( \epsilon_0 \) might be discontinuous between \( Y_f, Y_b, Y_g \), and \( Y_s \). To put it in a nutshell, we have to substitute (2.9) by

\[
\begin{align*}
- \nabla \cdot (\epsilon_0 \nabla \Phi) &= \rho_e + \delta \rho_{e}^{rs} \quad \text{in} \quad (0, T) \cap Y, \\
E &= -\epsilon_0 \nabla \Phi \quad \text{in} \quad (0, T) \cap Y, \\
\int_{Y} \Phi \, dx &= 0 \quad \text{in} \quad (0, T),
\end{align*}
\]

with scaling factor \( \delta = 1 [L^{-1}] \). (2.8) and (2.11) is called the Nernst–Planck–Poisson equation with sub-dimensional sources (NPPSS equation). The sub-dimensional sources are represented by \( \rho_{e}^{rs} \) which is the total charge density on the solid blocks’ faces and — from a mathematical point of view — a \( \delta_{d-1} \)-distribution.
The new consistency condition can be formulated as

\[ \int_Y \rho_e \, dx = - \int_{\Gamma_s} \rho_e^{rs} \, d\sigma, \]

that is, sources and sinks of the electric potential have to cancel out globally, or that the whole domain must be electrically neutral.

**Diffusion equations for molecules.** The evolution of the concentrations of uncharged molecules \( \omega^0 \) (which are only present in \( Y_f \cup Y_b \)) and \( \omega^0 \) (which are present in fluid, bio, and gas cells) is described by diffusion equations being similar to (2.8) with \( C_r \equiv 0 \). For molecules which do not exist in the gas, this yields

\[
\begin{align*}
\partial_t \omega^0_r - \nabla \cdot (D_r \nabla \omega^0_r) &= R_r \quad \text{in} \quad (0, T) \otimes (Y_f \cup Y_b), \\
G_r(\omega, \partial_t \omega, \omega^f, \partial_t \omega^f) &= 0 \quad \text{on} \quad (0, T) \otimes \Gamma, \\
- (D_r \nabla \omega^0_r) \cdot \nu &= \partial_t \omega^0_r \quad \text{on} \quad (0, T) \otimes \Gamma, \\
- (D_r \nabla \omega^0_r) \cdot \nu &= 0 \quad \text{on} \quad (0, T) \otimes \Gamma_{LG}, \\
\omega^0_r &= \omega^0_r \quad \text{in} \quad \{0\} \otimes (Y_f \cup Y_b),
\end{align*}
\]

while molecules that also exist in the gas phase have to satisfy Henry’s law on \( \Gamma_{LG} \):

\[
\begin{align*}
\partial_t \bar{\omega}_r^0 - \nabla \cdot \left( D_r \nabla \bar{\omega}_r^0 \right) &= R_r \quad \text{in} \quad (0, T) \otimes (Y \setminus Y_s), \\
G_r(\omega, \partial_t \omega, \omega^f, \partial_t \omega^f) &= 0 \quad \text{on} \quad (0, T) \otimes \Gamma, \\
- (D_r \nabla \bar{\omega}_r^0) \cdot \nu &= \partial_t \bar{\omega}_r^0 \quad \text{on} \quad (0, T) \otimes \Gamma, \\
\bar{\omega}_r^0 |_{Y_f \cup Y_b} / \bar{\omega}_r^0 |_{Y_g} &= H_{r \otimes \Gamma_{LG}} \quad \text{on} \quad (0, T) \otimes \Gamma_{LG}, \\
\left( D_r \nabla \bar{\omega}_r^0 \right) |_{Y_g} \cdot \nu_g - \left( D_r \nabla \bar{\omega}_r^0 \right) |_{Y_f \cup Y_b} \cdot \nu_g &= 0 \quad \text{on} \quad (0, T) \otimes \Gamma_{LG}, \\
\bar{\omega}_r^0 &= \bar{\omega}_r^0 \quad \text{in} \quad \{0\} \otimes (Y \setminus Y_s).
\end{align*}
\]

### 2.2.3 Cellular automaton method

A redistribution of solid, bio, and gas cells is defined according to restructuring / spreading / reorganizing rules — based on the evaluation of stencils (cf. Figure 2.3) — as presented in the following and the fluid cells are their remainder. The rules of the CAM are described in two spatial dimensions and for building units consisting of exactly one cell only, but they are analogously defined in three dimensions and for bigger building units.
**Biomass spreading rule.** The *biomass spreading rule* is implemented similarly to CAM CA-3 described in [33] and to the CAM as outlined in [35]. In summary, it can be described as follows: In each time step the bio cells $Y_b^i$ are identified where the mean biomass concentration exceeds its threshold value $\int_{Y_b} c_{B,\text{max}} \, dx$. For all these cells (*center cells*), the neighboring fluid and bio cells are tested whether they may take up a certain amount of excess biomass. These evaluations are executed in a random order. In doing so, a *shortest path strategy* is applied. More precisely, the cells belonging to the *stencil* of size 1 (■ in Figure 2.3) are investigated first. If necessary, thereafter, the stencil of size 2 (□ in Figure 2.3) is taken into account. If these stencils are not sufficient, the size of the stencils is incremented step-by-step to find possible target cells. Of these potential *target cells*, the closest ones are incrementally chosen to take up the excess amount of biomass. If several of the closest candidates are available, the one with the highest capacity is chosen. If more than one such target cell is identified, one is randomly chosen.

If the selected target cell may not take the complete amount of excess biomass the procedure described above is applied repeatedly. This results in the fact that the excess amount of biomass is potentially distributed to several target cells, each taking a certain part of the overall excess amount of biomass. Finally, if no additional target cell can be found, the amount of biomass is altered to its maximum value in the center cell, and the rest is discarded.

The redistribution of biomass is repeated until no biomass cell exceeds its threshold value or all cells have reached the maximum amount of biomass.
Note that there also are other (justified) rules for biomass spreading in the literature, for example, biased spreading to cells with the highest nutrient concentrations. Moreover, the “discarded” biomass needs to be justified. In some other models with biomass spreading via the CAM approach (e.g. [35]), there is bulk advection of the fluid phase and it is plausible that biomass can be removed from the system. In the current study, there is only diffusion and the “discarded” biomass is justified by the assumption that a lack of space deteriorates the biomass growth (but not the consumption of nutrient, etc.). For that reason the excess biomass is supposed to never have existed (within the model) which is corrected within the CAM.

**Solid restructuring rules.** The restructuring rules for solid cells are inspired by [18]. However, in [18] the stability of “particle clusters” is calculated by “summing over the affinities of particle–particle bonds”. Afterwards the 1% of weakest clusters is selected and one cell per cluster is redistributed, whereas we proceed as follows:

In each time step, “single” solid cells are identified, i.e. cells (or bigger inseparable building units) that are not bound to either biomass or further solid by either gluing agent or electric forces. More precisely, a “single” solid block $\hat{Y}_s^i$ potentially has certain biomass neighbor cells $Y_b^j$ as long as no gluing agent is present between them and certain solid neighbor cells $Y_s^k$ as long as (for some proportional constant $\gamma > 0$)

$$\int_{\partial Y_s^i \cap \partial Y_s^k} c_{a,i,k} - \gamma \rho_e^i Y_s^i \rho_e^k Y_s^k \mathrm{d}\sigma \leq 0. \quad (2.12)$$

Here, $\rho_e^i Y_s^i$ and $\rho_e^k Y_s^k$ denote the total charge densities of ions attached to $Y_s^i$ and $Y_s^k$, respectively. Thus, their integrated product tells whether two cells are bound to one another by electric forces or not. Moreover, $Y_s^i$ may have a gluing agent on its solid–fluid or solid–gas interfaces. In this sense “single” cells have the ability to move, since they are not bound to any other model component. Note that attraction means a positive contribution to the left-hand side of (2.12) by gluing agent concentration or electric forces stemming from charge densities with opposite signs. On the other hand, electric repulsion means negative contribution from the second term for charge densities with the same sign.

With the gluing agent possibly decaying in time, composites may break up again. The break up particularly happens if electrostatic repulsion becomes predominant in comparison to the gluing properties. Because of this, the counterbalance of electric forces and gluing properties on common faces of neighboring
solid cells $Y^k_i$ changes such that (2.12) turns from false to true (and makes the cell a “single” cell).

The attraction or affinity $A^i$ measures the potential of the $i$-th fluid or gas cell to attract a solid cell (and is defined as a weighted superposition of the different attracting and repulsing forces related to gluing agent, type of neighbors, and electric forces). It is evaluated in fluid and gas cells within a stencil — whose size might depend on the charge, volume, etc. of the “single” building unit — of neighboring cells (possible target cells) and for the “single” cell (center cell) itself:

$$A^i = \hat{\gamma} \left( \sum_{\text{neighbors} \neq Y^i_s} \int_{\partial Y^i_s \cap \partial Y^i_s} c_{\alpha,ij} \, d\sigma \right) + \text{number of solid neighbors} \neq Y^i_s \text{ of } Y^i_i$$

$$- \tilde{\gamma} \min \left\{ \sum_{\text{neighbors} \neq Y^i_s} \int_{\partial Y^i_s \cap \partial Y^i_s} \rho^e \tilde{Y}^s \rho^e \tilde{Y}^i \, d\sigma \right\} \quad \text{if } \tilde{Y}^i_s \text{ is a rotation of } Y^i_s \right\} (2.13)$$

with proportional constants $\hat{\gamma}$, $\tilde{\gamma}$, and $i$ denoting the index of a cell contained in the stencil around the center cell (cf. Figure 2.3). Rotations of solid cells relative to each other may become prominent in the case that not all of their faces are equally charged. With this definition, a relocation into favorable positions (as can be seen for $\odot$ in Figure 2.4) is facilitated.

Then, the target grid cell $Y^i_j$ with the largest $A^i$ is selected. If more than one such target cell is identified, one is randomly chosen and the restructuring is carried out. Note that this entails the exchange of a solid and a fluid/gas cell including all their properties such as nutrient and bacteria concentration within the grid cell.

A conflict may occur if the same target cell is selected by different solid center cells. To resolve such conflicts one solid cell is randomly chosen to jump to the respective target cell for each of the conflicts. The possible restructuring of the remaining solid cells is postponed to subsequent time steps. Likewise, bigger building units — cf. $\Box$ in Figure 2.1 — or larger agglomerates of building units are identified and the same procedure is applied as before.

In Figure 2.4 the reorganization of a charged solid phase is illustrated. A stencil of width two, cf. Figure 2.3, is applied to all solid cells. The arrows on the left hand side in Figure 2.4 indicate potential target cells for such a stencil. The continuous arrows indicate the jump to the most favorable positions for the
Figure 2.4: Effects of charges in solid restructuring. Initial configuration with potential movements to target cells (left) and consolidated configuration following the strongest attraction for each particle (right).

respective center cells. Dashed arrows indicate further possible and advantageous movements, while dotted arrows indicate disadvantageous movements. Moreover, bold-lined boundaries are assumed to be negatively charged, while dotted-lined boundaries are positively charged, and solid-lined boundaries are uncharged. Gluing agent is supposed to be absent in this illustration. On the right hand side in Figure 2.4, the final consolidated configuration is shown, after the cells have moved in alphabetical order. (The order of movement can have impact on the final configuration and is supposed to be randomly determined in numerical experiments.) The effect of charges is clearly visible: The solid cell denoted with \( C \) rotates in such a way that faces with opposite charges attach to one another and their charges balance out. Along this line, the absolute net charge of the system decreases, while electro-neutrality is preserved. The uncharged solid cell \( D \) moves in such a way that it obtains the maximal possible number of neighboring solid cells. Afterwards, the optimal position for \( E \) is its current position, since equally charged cells repulse each other.

**Reorganization rules for gas.** The *gas phase* is supposed to implement the fact that microaggregates are usually not completely filled with water. Hence, some dissolved (*aqueous*) chemical species and bacteria diffuse less easily through the pore space since they cannot cross the fluid–gas or bio–gas interfaces. They might even be physically entrapped by solid blocks on the one hand and gas blocks on the other hand. Contradicting, oxygen and other species present in the gas, the bio, and the fluid phases become more mobile since their diffusivities
are higher within gas cells. In natural soils the liquid (fluid and bio) phase is the wetting phase and the gas phase is the non-wetting phase. For that reason fluid and bio cells try to attach to solid cells while gas cells do not want to be direct neighbors of (have a common interface with) solid cells. That is, the solid cells are supposed to be “covered” by liquid cells.

In terms of the cellular automaton method, this can be implemented as follows: Whenever a gas cell has a common interface with a solid cell it evaluates its direct neighbors, i.e. a stencil of size 1 is applied (cf. Figure 2.3). If there is only one liquid neighbor of the gas cell (like it is for G in Figure 2.5) the gas cell and the liquid cell switch places. If there are several fluid/bio cells who are neighbors of the gas cell, one of the fluid/bio cells with the minimum amount of common interfaces with the solid phase is chosen to switch places with the gas cell. According to this rule fluid and bio cells attach to solid cells while gas cells do not.

Note that — like it is for relocating solid cells — this entails the exchange of a gas and a liquid cell including all their properties. A conflict may occur if the same target cell is selected by different gas cells. To resolve such conflicts one gas cell is randomly chosen to jump to the respective target cell for each of the conflicts. The possible reorganization of the remaining gas cells is postponed.
Figure 2.6: CAM including the reorganization of the gas phase illustrating its non-wetting property. Random initial configuration (left) and final configuration (right) with black solid, white gas, and gray fluid.

To subsequent iterations of the above procedure which is repeated till there are no common interfaces between the gas and the solid phases left or a maximum iteration number is reached.

In Figure 2.6 the functionality of the CAM is illustrated with focus on the reorganization of the gas phase and its non-wetting property on a computational domain consisting of $64 \times 64$ cells. A random configuration of solid (black), fluid (gray) and gas (white) cells with a volume proportion of 33% each is taken as starting point. After the CAM is run, it is evident that the fluid forms a film on the consolidated solid phase and liquid bridges can be found. Contrarily, the gas phase clearly shows its non-wetting property. However, there are some gas “bubbles” entrained by fluid, which may not be realistic. Thus, a further improvement of the CAM for the gas phase might be necessary in the future.

### 2.2.4 Upscaling rules and model characteristics

Finally, we attempt to evaluate the effect of the aforementioned mechanisms on characteristic properties of the porous medium such as porosity and an effective diffusion tensor. Hereby, we focus on the role of the solid’s restructuring and geometrical changes induced by biomass growth.

In order to evaluate the porosity $\theta$, the liquid porosity $\theta_{\text{liquid}}$, and the fluid porosity $\theta_{\text{fluid}}$, we calculate the time-dependent volume of the fluid domain $Y_f$, fluid–bio domain $Y_f \cup Y_b$, and fluid–bio–gas domain with respect to the total volume.
of the reference element $Y$:

$$
\theta_{\text{fluid}} = \frac{|Y_f|}{|Y|}, \quad \theta_{\text{liquid}} = \frac{|Y_f \cup Y_b|}{|Y|}, \quad \theta = \frac{|Y_f \cup Y_b \cup Y_g|}{|Y|}.
$$

(2.14)

**Upscaling of diffusion for aqueous molecules.** We hypothesize that the diffusion tensor for any diffusing (uncharged) species that only lives in $Y_f \cup Y_b$ may be determined via

$$
D_{ij} := \frac{1}{|Y|} \int_{Y_f \cup Y_b} D_{O_2/Bac/r,f,b}(\partial y \cdot \zeta_j + \delta_{ij}) \, dx
$$

(2.15)

with supplementary cell problems in $\zeta_j$, $j = 1, \ldots, n$

$$
\begin{cases}
-\nabla \cdot (\nabla \zeta_j + e_j) = 0 & \text{in} \quad Y_f \cup Y_b, \\
(\nabla \zeta_j + e_j) \cdot \nu = 0 & \text{on} \quad \partial(Y_f \cup Y_b), \\
\int_{Y_f \cup Y_b} \zeta_j \, dx = 0.
\end{cases}
$$

(2.16)

Hereby, $e_j$ denotes the unit vector in direction $j$ and $r$ is the index of the $r$-th molecular species only present in $Y_f \cup Y_b$. This result is well known in periodic settings and may be derived in such situations by means of asymptotic expansion. More details about this can be found in Chapter 3.

For the sake of simplicity, $D_{O_2/Bac/r,f} = 1$ and $D_{O_2/Bac/r,b} = 0.2$ in the following. This formula is, however, only strictly valid for periodic pore-scale geometries. Alternatively, one could approximate the upscaled diffusion coefficient by running a steady state simulation with a unit concentration gradient imposed as boundary conditions.

**Model characteristics.** Trying to compare the results of different executions of our numerical experiments we define characteristics that enable us to gain specific (and comparable) data about the properties of the generated aggregates. To do so, note that the word particle describes an insulated set of solid cells, i.e. a connected space of solid that cannot be further enlarged, in the following. The words agglomerate and composite describe a particle consisting of more than one inseparable building unit. The characteristics are related to the solid phase and given as:

- the total volume defined as the sum of the volumes of all solid particles, which is kept constant during our simulations. The total volume of composites defined as the sum of the volumes of all composites (where the volumes of singular building units is neglected) increases when single building units form composites.
2.3 Algorithm and implementation

The equations of the continuum model part are discretized using the local discontinuous Galerkin method, as described in Chapter 5, Section 2.B, and [9, 10] on the grid of quadratic (cubic) cells which is naturally induced by the model formulation (cf. Figure 2.1). The lower dimensional source terms are incorporated as symmetric flux corrections (see Section 2.B). The used discretization of Henry’s law can be found in Section 5.2 and [10]. Finally, the fully discrete system of equations is obtained via an approximation of the time-derivative by the first order backward difference quotient, i.e. we apply an adaptive, implicit Euler
\[ t = 0, \bar{t} = \bar{\bar{t}} \]

While \( t < T \)

<table>
<thead>
<tr>
<th>NUMITER = 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Do While the residual of NLSE is ( &gt; \epsilon_1 ) and NUMITER &lt; MAXITER</td>
</tr>
<tr>
<td>Continuum model component: Solve PDEs, ODEs, AEs which are introduced in Section 2.2.2, i.e. ensure that the residual of NLSE is ( &lt; \epsilon_2 ).</td>
</tr>
<tr>
<td>Continuum model component: Execute the transformation rules for a fluid cell turning into a bio cell as described in Section 2.2.2, i.e. update the geometric structure.</td>
</tr>
<tr>
<td>Compute the residual of NLSE with the new geometric structure.</td>
</tr>
<tr>
<td>NUMITER = NUMITER + 1.</td>
</tr>
</tbody>
</table>

If the residual of NLSE is \( < \epsilon_1 \) and \( \bar{t} = t + \tau \)

| Discrete model component: CAM for biomass spreading, i.e. update geometric structure. |
| Discrete model component: CAM for solid restructuring, i.e. update geometric structure. |
| Discrete model component: CAM for reorganization of gas phase, i.e. update geometric structure. |
| \( t = t + \bar{\bar{t}} \). |

If the residual of NLSE is \( < \epsilon_1 \)

| Possibly compute characteristic properties in current geometry (LDG). |
| \( t = t + \tau \) and \( \tau = t - \bar{t} \). |

If the residual of NLSE is \( \geq \epsilon_1 \)

| Repeat time-step with \( \tau = \tau/2 \). |

Table 2.1: Algorithm for the discrete–continuum model.

scheme with time-step restrictions raised by the Nernst–Planck equations. These restrictions occur since e.g. the Nernst–Planck equations are a set of non-linear equations and Newton’s method only ensures local convergence for the resulting non-linear system of equations (NLSE). If the time-step is too large the initial iteration might be too far away from the solution.

The overall algorithm including the continuum model part and the CAM is depicted in Table 2.1 and in Figure 2.21 on page 75, where \( t \) is the old time-step, \( \tau \) denotes the time-step size, \( \bar{t} \) is the current or next time when the CAM is evaluated (respectively), \( T \) is the end time of the simulation, and MAXITER, \( \epsilon_1 \),
$e_2$ are constants. The frequency of updates of the geometric structure (defined by $\tilde{\tau}$) has an important impact on the evolution of the domain and thus has to be related with realistic time intervals in an non-artificial simulation. In [35] twice a day is chosen. A second time stepping $(t, \tau)$ is introduced for operator splitting between the different types of models in Section 2.2, but in numerical experiments we most often recognized that $\tau = \tilde{\tau}$.

Within the discrete model component — which is solved for all global time steps — the main factors related to structural changes, apart from the generation of biomass from bacteria, are investigated, namely the biomass spreading, the solid restructuring, and the gas reorganization. Thereafter, characteristic time-dependent properties such as porosity and effective diffusion tensor are possibly evaluated.

The simulation software was completely implemented in M++ [43] for the fully implicit version of the scheme and uses MPI parallelization for the PDE and the CAM parts of the model. The CAM part of the model induces much communication between different processors (especially for larger stencils). Conflict resolution strategies have to be incorporated if different cells have the same target location and jumps over processors’ boundaries are necessary. In general, it turned out that the computational effort of the CAM increases drastically (compared to the effort for solving the PDEs) if the portion of solid is high and large stencils are applied. Moreover, wide parts of the model are also implemented in MATLAB 2016a\(^1\) using an additional operator splitting of the transport from the reaction parts of the respective equations.

### 2.4 Simulation scenarios and model evaluation

To the best of my knowledge, this research combines for the first time geometric changes resulting from biomass development, solid restructuring, and gas reorganization within a sophisticated multi-dimensional numerical discretization. Likewise, bridging scales in this context has rarely been done in other research and is another focus of the work. In one dimension and a simpler model framework without homogenization [40] investigates similar effects as done here.

Furthermore, different simulation and upscaling scenarios are evaluated. At first, the structural changes originating from biomass growth and decay, or from the restructuring of the solid, are illustrated separately, see Section 2.4.1 and Section 2.4.2, respectively. Particular attention is paid to the impact of the

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underlying structure on the effective diffusion tensor as defined in (2.15). In summary, it can be said that altering the pore space leads to a significant change in the medium’s characteristic properties.

To demonstrate the impact of the implemented mechanisms on the formation of structures in soils, several simulation scenarios are presented. The first scenarios focus on the demonstration of single effects and are chosen in such a way that the self-organization according to CAM rules is illustrated. To this end, various model components such as charges, biomass, gluing agent, or solutes in the liquid, etc. are switched off. Thereafter, combined effects are investigated to illustrate the overall capability of the model. Finally, the interplay of discrete and continuum model components is shown.

For all simulation scenarios, periodic conditions are prescribed on the square’s boundary $\partial Y$. Moreover, we assume that there are no external sources of nutrient, biomass, solid, or bacteria within the domain.

### 2.4.1 Effects of biomass development on effective diffusion

In this section, the impact of biomass development on the effective diffusion tensor defined in (2.15) is illustrated.

As depicted in Figure 2.7, the square $Y$ consisting of $16 \times 16$ fluid cells is considered. Throughout the simulation no solid is present. Initially, the nutrient distribution in the fluid has a parabolic profile in the horizontal direction and is
constant in the vertical direction, i.e.
\[ c_{O_2}(x, y, 0) = 100 \cdot x \cdot (1 - x) \, [N/L^2], \quad (x, y) \in (0, 1)^2. \quad (2.17) \]

In the middle of the domain \( Y \) a considerably high concentration of bacteria \( c_{Bac} = 20 \, [N/L^2] \) (particularly above the threshold value \( c_{Bac,\,\text{max}} = 10 \, [N/L^2] \)) covering \( 4 \times 4 \) cells is prescribed. Here, and in the following \( c_{B,\,\text{min}} = 0 \, [N/L^2] \) and \( c_{B,\,\text{max}} = 100 \, [N/L^2] \). The relevant constants for this scenario are: \( \text{const}_1 = 10, \, k_{d,B} = 0.1, \) and \( \text{const}_6 = 1/3. \)

The picture and effective diffusion tensor on the left in Figure 2.7 indicate that biomass is initially absent within the whole domain and that the diffusion tensor is equal to the identity naturally representing free diffusion.

According to (2.3a) and the CAM described in Section 2.2.3, a biomass is developing from bacteria and grows, as seen in the middle picture in Figure 2.7. The porosity values as defined in (2.14) develop as follows: The porosity \( \theta_{\text{fluid}} \) for the fluid decreases drastically from \( \theta_{\text{fluid}} = 1 \) to \( \theta_{\text{fluid}} = 0.710 \) and then to \( \theta_{\text{fluid}} = 0 \), whereas the total porosity \( \theta \) for the bio and fluid cells must remain constant (\( \theta = 1 \)) throughout this simulation. Moreover, the eigenvalues of the effective diffusion tensor reasonably decrease, see the tensors in Figure 2.7. This is due to the fact that diffusion is significantly lower (reduced by 80%) in the bio cells compared to the fluid.

Finally, as depicted in the picture on the right in Figure 2.7, biomass has grown substantially and covers the whole domain. As expected, the eigenvalues of the diffusion tensor are equal to 0.2. It is remarkable that this value is independent of the biomass concentration and only depends on its occurrence, potentially in relation to the occurrence of a fluid or solid.

As oxygen is the main driving force and completely consumed in the long run, the initial state equals the final stationary state (not depicted here).

### 2.4.2 Effects of gluing agent dominated solid restructuring on the effective diffusion tensor

As a second example, we evaluate the reorganization of solid cells due to the restructuring rules as described in Section 2.2.3 and their impact on the effective diffusion tensor as defined in (2.15).

As illustrated in Figure 2.8 the square \( Y \) consisting of \( 16 \times 16 \) cells is considered. The initial distribution of solid cells (red) and its remainder — the fluid — are randomly chosen. The initial nutrient distribution obeys (2.17), except for the domain of the solid, see picture on the left in Figure 2.8. Note that neither bacteria, ions nor gas or bio cells are present in this scenario, and that \( k_{d,\alpha} = 0.3, \, \text{const}_3 = 10, \) and \( \text{const}_5 = 0.5. \)
Throughout the simulation scenario (2.1) and (2.4) are solved. Moreover, the solid restructuring rules as described in Section 2.2.3 are applied. This results in a redistribution of the solid cells due to gluing agent consuming nutrient and thereby growth of the gluing agent, but also due to the lack of the nutrient and the degradation of gluing agent as time proceeds. In Figure 2.8, the structural changes of the solid are depicted. After the first global time steps, nutrient has diffused and been consumed within the pore space, which has been altered due to the restructuring rules and the evaluation of (2.13); see picture in the middle of Figure 2.8. In addition to the movement of single cells, it is evident from Figure 2.8 that double-blocks have rearranged.

Due to the absence of growing or decaying biomass, the porosity of the sample has the fixed value 0.6914. The diffusion tensor alters due to the alteration of the pore space and is computed according to (2.15), cf. Figure 2.8.

Since we have no sources for nutrient in this scenario, nutrient is diffusing and being consumed in the long run, and consequently also the movement of solid particles tends to a quasi stationary state where still some solid cells may jump to equally favorable positions, but bigger agglomerates are not allowed to move here.

**Influence of the domain size.** Interestingly, the size (or number) of the particles in our domain $Y$ seems to have no significant effect on the effective diffusion tensor or its eigenvalues (as long as porosity is kept constant). This is further demonstrated by simulations prescribing the same porosity and consisting of...
2.4 Simulation scenarios and model evaluation

\begin{figure}[h]
\centering
\begin{tabular}{cccc}
0.303, 0.455 & 0.354, 0.405 & 0.312, 0.380 & 0.347, 0.355 \\
(0.390, 0.075) & (0.399, 0.015) & (0.319, -0.021) & (0.354, -0.001) \\
(0.075, 0.368) & (0.015, 0.359) & (-0.021, 0.373) & (-0.001, 0.347) \\
\end{tabular}
\caption{Evolution of solid (black), diffusion tensor $\mathbb{D}$, and eigenvalues $\lambda_i$ for domains $Y$ consisting of $10 \times 10$, $20 \times 20$, $50 \times 50$, and $100 \times 100$ cells (from left to right).}
\end{figure}

$10 \times 10$, $20 \times 20$, $50 \times 50$, or $100 \times 100$ cells in the domain $Y$. Figure 2.9 shows the quasi stationary states, diffusion tensors, and eigenvalues for these four different configurations at $t_{\text{end}} = t_{200}$. The solid always coalesces in (several) not necessarily rectangular bigger blocks in the quasi stationary limit. This coalescence is due to the fact that the second term in (2.13) (number of neighbors) dominates the impact of the degrading gluing agent. However, the bigger aggregates may not coalesce further in this setting due to the definition of the stencil, compare Figure 2.3, and the fact that agglomerates are not allowed to move in this scenario.

**Degeneration of homogenized tensors.** The supplementary cell problem for homogenization has proven to potentially be ill posed for certain time steps, i.e. when the system matrix is close to singular. This is due to the fact that

\begin{figure}[h]
\centering
\caption{Geometry of (black) solid leading to degenerated diffusion tensor.}
\end{figure}
insulated fluid or biomass cells appear (e.g., one single fluid cell and a pair of fluid cells in the center of the computational domain depicted in Figure 2.10). In such a situation the pore space is no longer connected and the underlying mathematical problems (2.16) are not uniquely solvable. Such situations become more probable as the porosity \( \theta \) decreases. However, restructuring of the solid and coalescing into bigger solid blocks may in turn lead to a connected pore space for which the upscaled diffusion tensors are again well defined.

**Influence of coincidence.** As a next step, we investigate the influence coincidence has on the calculated diffusion tensors. In doing so, we consider the square \( Y \) of \( 16 \times 16 \) cells in which initially an U-shaped solid as shown in the picture on the left of Figure 2.11 is prescribed. Moreover, initially no biomass is present. The initial bacteria and also the nutrient concentration have a parabolic profile in the horizontal direction and are constant in the vertical direction, cf. (2.17). Since biomass and bacteria have vanished in the quasi stationary states and the focus lies on the development of the diffusion tensor, their development is not illustrated here.

The same simulation was repeated 100 times. Exemplarily, four stationary states are shown in Figure 2.11. Moreover, the eigenvalues of the 100 simula-
Evolution of eigenvalues of homogenized tensors. Pertaining to the influence of porosity on the eigenvalues of the computed diffusion tensors, we consider the same situation as in the beginning of Section 2.4.2 (up to the initially randomly chosen distribution of the solid).

The resulting (time-dependent) diffusion tensors’ eigenvalues are displayed in Figure 2.13. Here, the eigenvalues at the time of initiation are depicted in red, while the eigenvalues after 50 global time steps are depicted in blue. The dashed and dotted lines represent the larger and smaller eigenvalues, respectively. In summary, the eigenvalues increase as time proceeds. This means that the restructuring of the solid facilitates diffusion due to the consolidation of larger solid blocks (compare the first example of Section 2.4.2). Likewise, the values increase considerably with an increasing porosity and have a peak at \( \theta = 1 \) representing free flow. A more elaborate evaluation of this effect can be found in Chapter 3.

2.4.3 Combined effects of biomass development, gluing agent, and solid restructuring on the diffusion tensor

This versatile and complex model — combining the effects of many processes — can, e.g. map the interplay of dynamic biomass depending on the availability
of nutrients and its consequences on the aggregation of solid particles linked by dynamic gluing agent. This may also lead to an entrapment of solid particles by surrounding biomass. (Simulations not shown here, but can be found in [2, p.
In the following example, we focus on the impact of the structural changes on the effective diffusion tensor as defined in (2.15).

As illustrated in Figure 2.14 the square $Y$ consisting of $16 \times 16$ cells is considered. The initial distribution of solid cells is randomly chosen. Initially no biomass is present. The initial bacteria and nutrient concentrations obey (2.17), see pictures on the left in Figure 2.14.

The distribution of the solid (which is depicted red in the bottom line) results in an effective diffusion tensor that has zero as an eigenvalue. This indicates that diffusion is possible from bottom to top, but is not possible from left to right (remember the periodic boundary conditions to $\partial Y$).

After the first global time steps, only few solid blocks have moved, since bacteria have transformed into biomass. This biomass has nearly filled the complete pore space and inhibits movement (see the second column in Figure 2.14). Moreover, due to the availability of the nutrient, the solid cells are additionally held together by gluing agent.

The computation of the effective diffusion tensors shows the behavior that is expected for such a setting: The eigenvectors (principle directions of diffusion) and the eigenvalue equal to zero remain fixed, since the solid has not changed its structure significantly and biomass has filled almost the complete pore space. Yet the other eigenvalue $\lambda_1$ decreases significantly from $0.3240 \, [L^2/T]$ to $0.0749 \approx 20\% \cdot 0.3240 \, [L^2/T]$ due to the fact that diffusion is significantly lower (reduced by 80%) in the biomass compared to the fluid, compare Section 2.4.1. This indicates that diffusion is still dominant from bottom to top, and is not possible from left to right.

As can be seen in the pictures on the right in Figure 2.14, after 50 time steps the biomass has decayed completely again due to the lack of oxygen. This enables the restructuring of the solids and — like in Section 2.4.2 — larger solid blocks have formed. As can be deduced from the corresponding diffusion tensor in Figure 2.14, diffusion is now also possible from left to right.

### 2.4.4 Effects of the range of attraction

Now, we investigate the influence of the range of attraction of particles (which is represented by different stencil widths) on each other for structure formation. Since this scenario focuses on the demonstration of a single effect, no charges, biomass, gluing agent, or solutes in the liquid etc. are taken into account. Thus, attraction of the cells to each other is uniform and can be interpreted as the sum of attracting forces as, e.g. *van der Waals* forces, that also lead to *homoaggregation*. It is thus only determined by the number of neighbors (see eqn. (2.13) with $\bar{\gamma} = \bar{\gamma} = 0$). Initially, a domain with 50% solid cells and 50% fluid cells and $256 \times 256$ cells in total is randomly created and any charge effects are disregarded.
From this initial configuration (cf. picture on the left in Figure 2.15) the CAM is run with a stencil of width 1 [L] and with a stencil of width 3 [L], cf. Figure 2.3. Note that agglomerates are allowed to move in this section.

Since we study the formation of structures and do not consider their disaggregation here, the simulations run into a quasi-stationary state. The resulting aggregated structures are depicted in the middle of Figure 2.15 (for a stencil of width 1) and in the right of Figure 2.15 (for a stencil of width 3). It is evident that the self-organization of the solid phase highly depends on the range of attraction represented by the size of the stencil. A smaller range of attraction leads to finer structures, i.e. higher specific surface areas of the solid phase (initially: $65168/32768 \approx 1.99$ [L$^{-1}$], stencil of size 1: $29720/32768 \approx 0.91$ [L$^{-1}$], stencil of size 3: $9208/32768 \approx 0.28$ [L$^{-1}$] after 500 CAM steps; cf. Figure 2.15). Contrarily, the larger range of attraction induces coarser, connected structures, and thus also the average size of the pore channels is larger (Figure 2.15, right).

Although the choice of the stencil width representing the range of electric forces can be determined quite well (see [29]), the analog of the attraction range originating from other forces such as gluing effects, has to be estimated. Our model allows to study such effects separately to validate related assumptions. Moreover, the combination of different effects on structure formation may also be studied in silico. In principle, each prototype of particle (cf. Figure 2.2) may have a different range of attraction depending for instance on its charge. This is represented in the model as an individual stencil size (see Figure 2.3) for each prototype of a particle.
2.4.5 Effects of the shape of building units

Shape and size of the inseparable building units strongly influence the formation of structural patterns. For an illustration of this effect, we consider domains of $256 \times 256$ cells where 50% are filled by uncharged solid building units (either single cells or needles of length 5). In Figure 2.16 the random initial configurations are shown on the left hand side. The corresponding quasi-stationary states (after 500 CAM steps) are depicted on the right hand side. (Note that the first row of Figure 2.16 is included in Figure 2.15.) For each simulation, a stencil of size 1 is applied to single building units and isolated agglomerates. It is evident that rearrangement and aggregation have occurred for both simulation scenarios which are, however, more prominent in case of the single cells. This is clearly due to size effects since the rearrangement of needles is physically restricted for quite high volume fractions of the solid. The small building units have more options to move to a free single cell, and thus create denser structures. Thus, less smooth structures are created for needles as compared to single cells and the specific surface has decreased less: for the the latter ones by a factor of 0.46.

Figure 2.16: Self-organization depending on shape and size constraints: Left: Initial random configuration with single solid cells (top) and needles (bottom) in black with porosity $\theta = 0.5$; right: quasi-stationary states with a stencil of 1.
(from initially 1.99 to 0.91 [L^{-1}]), and for the needles by a factor of 0.84 (from 46096/32768 \approx 1.41 to 38950/32768 \approx 1.19 [L^{-1}]).

2.4.6 Effects of charges

Electrostatic forces are a major driving force for particle aggregation, cf. [36]. Volume and surface charges lead to repulsion or attraction of particles (or faces). This effect is significantly different compared to the uniform attraction among particles as has been investigated so far. To depict this effect in more detail, we compare the following two simulation scenarios: For the same initial configuration and disregarding the role of charges (and other effects as a heterogeneously distributed gluing agent, e.g.), the uniform attracting forces lead to augmenting the number of neighbors in the first setting, cf. (2.13) with \( \hat{\gamma} = \overline{\gamma} = 0 \). Second, the effect of charges is additionally taken into account, i.e. \( 1 = \overline{\gamma} \neq 0 \).

As initial configuration, we consider 20% solid particles and 64 \times 64 cells in total. For the second scenario, we randomly distribute constant charge numbers between \(-4\) and \(+4\) on all solid cell faces \( \partial Y^i_s \). For each scenario, we run the CAM 200 times with a stencil of size 2 [L] for single building units and agglomerates, and evaluate the attraction according to (2.13). The simulation results are depicted in Figure 2.17. The quasi stationary states for the simulation scenarios without and with charge effects are shown in the middle and the right pictures of Figure 2.17, respectively. It is evident that the principle of augmenting the number of neighbors leads to quite large and blocky structures. In contrast to this, fine and dendritic structures, also called card-house structures, are obtained if charges are taken into account. This is due to the repulsion of particles with

Figure 2.17: Effects of charges in solid restructuring: Initial configuration for both simulations, porosity \( \theta = 0.8 \) (left), quasi stationary configuration without charges (middle), and quasi stationary configuration with randomly distributed charges dominating the restructuring (right).
equal charge. Such card-house structures are frequently observed in soils with clay particles (cf. [13]) and lead to three times higher specific surfaces (initially $\frac{2522}{819} \approx 3.08 \text{ [L}^{-1}]$, for uncharged particles $\frac{444}{819} \approx 0.54 \text{ [L}^{-1}]$, and for charged particles $\frac{1328}{819} \approx 1.62 \text{ [L}^{-1}]$), cf. Figure 2.17.

### 2.4.7 Effects of the electrostatic field in the solution

In this section, we combine the restructuring of phases according to the CAM with the PDE model for movement of potentially charged species in solution. Thus, we show the interplay of ions in solution that adsorb to charged particles, i.e. we combine the CAM for charged solids with the PDEs for a charged fluid phase. The adsorption of ions to the surfaces defined by

$$\partial_t \omega_{r}^{\Gamma, \pm} = k(g_{r}^{\pm} - \omega_{r}^{\Gamma, \pm}) = 1[T^1] \cdot \left( \frac{0.3[L]\omega_{r}^{\pm}}{[N]} + 0.3[L^2]\omega_{r}^{\pm} - \omega_{r}^{\Gamma, \pm} \right)$$

changes the attraction of particles and the resulting structures. The left picture in Figure 2.18 shows the initial state of a randomly distributed solid with randomly charged surfaces (charge numbers between $-4$ and $+4$) on a domain of size $32 \times 32$ with $D_r = 10^{-8} \text{ [L}^2/T]$, $C_r = 10^{-3} \text{ [T}^2/M]$, and the other physical constants set to one.

We compare the resulting structures under the influence of an uncharged chemical species and positively/negatively charged species. The uniform initial concentration of the uncharged species is $10 \text{ [N/L}^2]$ and homogeneous Neumann boundary is applied at the solid’s surface $\Gamma$. Likewise, the uniform initial concentration of the positively charged chemical species is set to $10 \text{ [N/L}^2]$. To ensure electro-neutrality (also balancing the total charge of the solid), a negatively charged species with an initially homogeneous concentration of $13.27 \text{ [N/L}^2]$ is necessary (not plotted in Figure 2.18). The middle and right image in Figure 2.18 depict the quasi stationary, consolidated configurations of the solid (after 100 CAM steps with a stencil size of 3 $\text{ [L]}$), when uncharged or charged species are considered, respectively. The inert uncharged species has remained constant at $10 \text{ [N/L}^2]$ as depicted in the middle picture of Figure 2.18. For the charged species heterogeneous reactions with the solid are included which alter the solid’s charge and thus also the structure formation. In the zoom in the right of Figure 2.18 we see high surface concentrations of the charged species near high concentrations in the solute, and vice versa. The altered surface concentrations by sorption have an impact on the attraction of the solid particles and thus on the resulting solid structure. This becomes evident when comparing the aggregated particles in the respective final states.
Figure 2.18: Interplay of ions in solution with charged solids: Initial configuration (first image) of solid (red), quasi stationary, final configuration of charged solid in neutral solution (second), and final configuration of charged solid in ionic solution (third image) when heterogeneous reactions alter the total charges of solid cells’ edges. The zoom highlights charges on solid edges, the rainbow scale corresponds to the surface concentrations.

Figure 2.19: Aerobic bacteria in fluid phase combined with solid restructuring and gas reorganization: The scale depicts the concentration of a nutrient. Thus, solid cells are red, fluid cells are violet to dark blue, and gas cells are pale blue to white in the right picture.
2.4.8 Effects of Henry’s law and gas phase

Next, we combine the restructuring of phases according to the CAM with the PDE model to illustrate the capability of our comprehensive model: A three phase system (as in Figure 2.6) is taken into account without any electric field or charges (33% solid, 33% fluid, 33% gas cells randomly distributed), cf. the picture on the left in Figure 2.19. Within the gas phase and the fluid phase a constant distribution of a species of 4 [N/L²] and 2 [N/L²], respectively, is present initially. It is degraded with a first order rate and rate constant $-0.375$ [1/T] in the fluid phase representing, e.g., the consumption of a nutrient, such as oxygen by aerobic organisms in the fluid phase. The diffusion is faster in the gas phase ($D = 10^{-4}$ [L²/T]) compared to the fluid phase ($D = 10^{-8}$ [L²/T]) and the transfer between the phases is determined via Henry’s law with solubility constant $H_{f,g} = 2 [-]$. The picture on the right in Figure 2.19 shows the resulting distribution of the phases and species after the PDEs for the species are solved and the CAM is run simultaneously (50 steps on a domain of 64 x 64 cells). It is evident that phase transfer determined by means of Henry’s law, leads to a jump in the nutrient concentration across fluid–gas interfaces and therefore to a non-uniform distribution of the nutrient in the pore space. Moreover, concentration gradients are visible in the fluid and gas phases which become more prominent for lower diffusivity. This leads to nutrient-poor and nutrient-rich regions within the created aggregate structure.

2.4.9 Hybrid multiscale model

We now illustrate the functionality of this modeling approach to take into account the impact of the microscopic on the macroscopic scale. In particular the effect which the underlying microstructure’s evolution has on macroscopic diffusion is investigated in a weakly coupled multiscale problem: We consider the following diffusion equation for a macroscopic concentration $c(t, x, y)$ in a macroscopic domain $\Omega$ (a square) with Neumann boundary conditions on $\partial \Omega$:

$$\partial_t c - \nabla \cdot (D \nabla c) = 0 \quad (x, y) \in \Omega, t \in (0, T),$$

$$D \nabla c(x, y, t) \cdot \nu = 0 \quad (x, y) \in \partial \Omega, t \in (0, T),$$

$$c(x, y, 0) = 10 \chi_{(1/4, 3/4)}(x, y) \quad (x, y) \in \Omega.$$

On the micro-scale, we refer to the example and diffusion tensors $D$ calculated in Section 2.4.3 and depicted in Figure 2.14.

Now the obtained time-dependent diffusion tensors that strongly depend on the underlying and changing geometry are integrated into the macroscopic diffusion problem. Note that this example is weakly coupled, i.e. back-coupling the...
Chapter 2  Model for microaggregate development

Figure 2.20: Evolution of macroscopic concentration at $t_1$ (left), $t_{50}$ (middle), and $t_{100}$ (right). The pictures have been generated with constant initial tensor (top), evolving tensor (middle), and constant final tensor (bottom).

The macroscopic diffusion equation’s solution onto the cell problems is not incorporated into the overall multiscale model. The macroscopic problem is discretized using linear finite elements and the software toolbox M++ [43].

In Figure 2.20, the following varying situations are illustrated: At the top row
of Figure 2.20, the initial singular diffusion tensor \( D_{O_2,t} = \begin{pmatrix} 0.000 & -0.000 \\ -0.000 & 0.324 \end{pmatrix} \) with first eigenvalue equal to zero from Figure 2.14 is taken for all times. In the middle row of Figure 2.20 the time-dependent diffusion tensor, i.e. starting with the singular matrix \( D_{O_2,t} = \begin{pmatrix} 0.000 & -0.000 \\ -0.000 & 0.324 \end{pmatrix} \) which becomes a symmetric positive definite matrix as time proceeds, is taken into account. At the bottom row of Figure 2.20 the final non-singular diffusion tensor \( D_{O_2,t} = \begin{pmatrix} 0.411 & -0.065 \\ -0.065 & 0.381 \end{pmatrix} \) from Figure 2.14 is considered for all times.

For the singular diffusion tensor (at the top row in Figure 2.20) a reasonably high concentration develops in the middle of the macroscopic domain whereas no concentration is present at the left and right sides. This is due to the fact that diffusion is strong in the vertical direction and not possible in the horizontal direction (first eigenvalue equal to zero).

Using the evolving diffusion tensors for all 100 time steps (unless it is badly scaled, cf. Section 2.4.2; middle, Figure 2.20), we obtain a concentration which behaves similar as before in the beginning. As time proceeds the concentration is high in the center of the domain and decreases considerably in the horizontal direction. Since the diffusion tensor turns into a symmetric positive definite matrix, meaning that diffusion is possible vertically and also horizontally, the concentration becomes more homogeneous after 100 steps (cf. the rescaled scale).

Turning now to the case that the final non-singular diffusion tensor is considered for all times, it can be deduced from the bottom row in Figure 2.20 that the diffusion occurs faster than in the previous cases since the diffusion is possible in all directions immediately from the beginning (no eigenvalue equal to zero) with considerably high eigenvalues compared to the evolving diffusion tensor.

### 2.5 Conclusions and future prospects

In this chapter, a comprehensive model for structure formation has been presented. A novel discrete–continuum approach was taken, combining a model of partial differential equations for charged, reactive multicomponent transport with a cellular automaton method for the interactive self-organization of solid, bio, fluid and gas phases. With the help of well-known results from homogenization theory the effects of these structural changes occurring on the micro-scale can be taken into account in macroscopic transport. Different processes leading to geometrical changes were incorporated and thoroughly illustrated by means of numerical simulations.
This versatile approach has the potential to study the interplay of different aggregation mechanisms \textit{in silico}. The systematic evaluation of a broad range of scenarios for microaggregate formation — also in comparison to batch experiments addressing aggregate formation — is subject of current work and a forthcoming article. It addresses, e.g., electrostatic shielding in realistic configurations, and studies structure formation at various concentrations and particle type relations.

The main purpose of the current research was to develop a tool to examine the strong interplay between functional properties and geometric structure even on larger scales. Although the results have already contributed towards enhancing our understanding of the impact of small scale processes and structures on a medium’s functionality, there are several levels of complexity that may be added to the model:

First, an extension to more elaborate multi-species \textit{biomass} and potentially also shrinking biomass as discussed in [33, 35] is possible along the lines of these publications. Second, more sophisticated \textit{reactions} and different types of \textit{nutrients} (e.g. oxygen and nitrate) could be integrated into the model.

Another necessary step in broadening further applications is the integration of (possibly unsaturated) fluid flow into our model. A \textit{pore-scale model} taking into account fluid flow and biofilm detachment by shear stress may be found in [35]. Here, biofilm development is calculated by means of a CAM. Likewise, in the context of upscaling, continuum fluid flow and biofilm models were considered in a thin strip in [38], in a locally periodic setting in [32], and in a geometry being extracted from the imaging data of glass beads inoculated with biomass in [31]. Combining such model extensions with the presented concept of solid restructuring seems to be quite promising for further investigations into the factors that affect soil’s functionality in the future.

Additionally, more research is needed to investigate unsaturated flow itself. This was for instance done for non-evolving angular \textit{pore networks} representing soil aggregates in [22]. Here continuum model approaches were combined with an individual based model for microbial community. The superposition of the results weighted with aggregate size distributions made it possible to access scales of practical interest. Traditional mathematical upscaling in unsaturated conditions has been performed in [20] to illuminate the parametrization of Richard’s equation. Likewise it is desirable to predict the \textit{water retention curve} in our setting. Moreover, the transport limited availability of nutrients and their role for \textit{habitat} could be investigated in further research. Such model extensions seem to be quite promising for further investigations of soil’s functionality in the future.

Furthermore, other process mechanisms could be identified. Those have to be
2.5 Conclusions and future prospects

determined and validated with the help of in vitro experimental studies which itself is a challenge. One step into that direction would be a model extension with respect to disaggregation of the resulting structures or the consideration of bulk advection of the liquid and gas phases. Different aggregation and disaggregation mechanisms and their respective ratios need to be investigated. Moreover, building units and their composites (i.e. smaller units of building units) naturally undergo some random movement (representing diffusion) independently of the CAM rules. Such a movement depending on the respective size of the particles needs to be included into the model.

A related research question is how time scales are related to diffusion and how interaction processes can be balanced in a reasonable way. In some other work in the literature (e.g. [34, 35]) that models reactive transport and biomass development, the authors claim that the time scales for reactive transport are short relative to the time scale of biomass development; this allows transport to be solved at steady state for a “frozen” solid configuration. The argumentation clearly has its beauty and is valid in a wide range of applications. Nevertheless, the thesis’ approach using parabolic equations from my point of view is slightly more general, since it poses the opportunity to “weight” (the impact of) different time scales and allows to investigate regimes where diffusive or reactive processes (possibly referring to larger spatial scales; cf. Chapter 4) are slow compared to discrete processes (which might be very local).

Finally, a quantitative evaluation of the resulting structures would be possible by means of Minkowski functionals and further geometric measures characterizing, among others, the connectivity and compactness of a structure. A first investigation of such a quantifying parameter (effective diffusion) is done in the next chapter. Beyond that, exploring the impact of different initial conditions for bacteria and gluing agent for simulations as done in Section 2.4.3 or imposing a gradient of the charged species in Section 2.4.7 and observing the effect on solid restructuring would be interesting.

Of course, this work is just a first step in modeling complex physicochemical processes in soil science, but it shows the way to a promising toolbox with versatile model components and is extendable to further process mechanisms. Those have to be identified and validated with the help of in vitro studies. This will be another future challenge.
### 2.A Appendix: Long formulas

<table>
<thead>
<tr>
<th>Cell states</th>
<th>Sticky agent</th>
<th>Cells’ alterations</th>
<th>Components</th>
<th>Components’ alterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>solid (s)</td>
<td>yes</td>
<td>restructuring</td>
<td>—</td>
<td>heterogeneous reactions (i.e. at-/detachment)</td>
</tr>
<tr>
<td>fluid (f)</td>
<td>not on f-f or f-g interfaces</td>
<td>passively movable</td>
<td>molec./ions</td>
<td>normal diffusion, possibly electric drift, homogeneous and heterogeneous reactions</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>nutrient (O\textsubscript{2})</td>
<td>normal diffusion, consumption by bacteria and gluing agent</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>bacteria (Bac)</td>
<td>normal diffusion, consumption of nutrient, transformation to biomass</td>
</tr>
<tr>
<td>bio (b)</td>
<td>yes</td>
<td>growing/shrinking</td>
<td>biomass (B)</td>
<td>nutrient consumption, generation from bacteria, growth and decay</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>molec./ions</td>
<td>weak diffusion, possibly electric drift, homogeneous and heterogeneous reactions</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>nutrient (O\textsubscript{2})</td>
<td>weak diffusion, consumption by biomass, bacteria, gluing agent</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>bacteria (Bac)</td>
<td>weak diffusion, nutrient consumption, integration to biomass</td>
</tr>
<tr>
<td>gas (g)</td>
<td>not on g-g or f-g interfaces</td>
<td>reorganizing</td>
<td>molecules</td>
<td>very strong diffusion, homogeneous and heterogeneous reactions</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>nutrient (O\textsubscript{2})</td>
<td>very strong diffusion, consumption by gluing agent</td>
</tr>
</tbody>
</table>

Table 2.2: Model parts.

\[
(\mathcal{f}_{\text{increase},t})_k(\mathcal{c}_{O_2}) = \begin{cases} 
0, & \text{if } \left( \int_{Y_k} c_{O_2} \, dx \leq \int_{Y_k} c_{up,O_2,\text{min},t} \, dx \right) \land \left( \int_{Y_l} c_{O_2} \, dx \leq \int_{Y_l} c_{up,O_2,\text{min},t} \, dx \right), \\
\text{const}_3, & \text{if } \left( \int_{Y_k} c_{O_2} \, dx > \int_{Y_k} c_{up,O_2,\text{min},t} \, dx \right) \land \left( \int_{Y_l} c_{O_2} \, dx \leq \int_{Y_l} c_{up,O_2,\text{min},t} \, dx \right) \lor \left( \int_{Y_l} c_{O_2} \, dx > \int_{Y_l} c_{up,O_2,\text{min},t} \, dx \right), \\
2\text{const}_3, & \text{if } \left( \int_{Y_k} c_{O_2} \, dx > \int_{Y_k} c_{up,O_2,\text{min},t} \, dx \right) \land \left( \int_{Y_l} c_{O_2} \, dx > \int_{Y_l} c_{up,O_2,\text{min},t} \, dx \right) 
\end{cases}, 
\] on $\partial Y_k \cap \partial Y_l$. (2.18)
Continuum model component:
- Solve PDEs, ODEs, AEs which are introduced in Section 2.2.2, i.e. ensure that the residual of NLSE is $< \epsilon_2$.
- Execute the transformation rules for a fluid cell turning into a bio cell as described in Section 2.2.2, i.e. update the geometric structure.
- Compute the residual of NLSE with the new geometric structure and set NumI = NumI + 1.

Discrete model component:
- CAM for biomass spreading, i.e. update geometric structure.
- CAM for solid restructuring, i.e. update geometric structure.
- CAM for reorganization of gas phase, i.e. update geometric structure.
- $\bar{t} = \bar{t} + \bar{\tau}$.

Figure 2.21: Flow chart illustrating the processes of Table 2.1.
2.B Appendix: A local discontinuous Galerkin scheme for different versions of the Nernst–Planck–Poisson equation

The NPP and NPPSS equations in Section 2.2.2 are discretized using the local discontinuous Galerkin method, as described in [9, 10] and Chapter 5. A similar discontinuous Galerkin scheme which induces less numerical diffusion since it requires smaller penalty terms is analyzed in [1]. For other types of discretization techniques the reader may consult [24, 25].

Firstly, a weak and mixed formulation of the respective equations is obtained by introducing an auxiliary flux variable \( q_r = -D_r V \omega_r^x \), multiplication of smooth, periodic test functions \( \varphi_\omega \) and \( \varphi_q \), \( \rho_\omega \) \( \rho_q \), and integration by parts. This yields for Equation 2.8 and all \( \varphi_\omega \in C^\infty \left( [0, T] \otimes Y_f \cup Y_b \right), \varphi_q \in C^\infty \left( [0, T] \otimes Y_f \cup Y_b \right) \)

\[
\int_0^s \left[ \int_{Y_f \cup Y_b} \left( \partial_t \omega_r^x \right) \varphi_\omega \, dx \right] + \int_{Y_f \cup Y_b} \left( C_r \omega_r^x E \right) \cdot \nabla \varphi_\omega \, dx - \int_{Y_f \cup Y_b} q_r \cdot \nabla \varphi_\omega \, dx + \int_\Gamma \left( \partial_t \omega_r^{\Gamma, x} \right) \varphi_\omega \, d\sigma - \int_{Y_f \cup Y_b} R_r \varphi_\omega \, dx \right] \, dt = 0, \tag{2.19a}
\]

\[
\int_0^s \left[ \int_{Y_f \cup Y_b} D_r^{-1} q_r \cdot \varphi_q \, dx \right] - \int_{Y_f \cup Y_b} \omega_r^x \left( \nabla \cdot \varphi_q \right) + \int_\Gamma \omega_r^x \varphi_q \cdot \nu \, d\sigma \right] \, dt = 0, \tag{2.19b}
\]

\[
\int_0^s \left[ \int_\Gamma \partial_t \omega_r^{\Gamma, x} \varphi_\omega \, d\sigma - k \int_\Gamma g \left( \omega_r^x \right) \varphi_\omega \, d\sigma + k \int_\Gamma \omega_r^{\Gamma, x} \varphi_\omega \, d\sigma \right] \, dt = 0, \tag{2.19c}
\]

\[
\int_{Y_f \cup Y_b} \omega_r^x (0, \cdot) \varphi_\omega (0, \cdot) \, dx - \int_{Y_f \cup Y_b} \omega_r (0, \cdot) \varphi_\omega (0, \cdot) \, dx = 0. \tag{2.19d}
\]

For simplicity of the notation, we assume that \( \Gamma := \partial Y_s = \partial Y_f \cap \partial (Y_f \cup Y_b) = \partial (Y_f \cup Y_b) \) and that there is no gas phase (i.e., especially no \( \Gamma_{LG} \), cf. Figure 2.1), here. The more general case can be dealt with analogously with gas cells treated like solid cells without any (volume or surface related) sources. Additionally, for Equation 2.9 and all periodic \( \varphi_\Omega \in C^\infty \left( \frac{Y_f \cup Y_b}{Y_f \cup Y_b} \right), \varphi_E \in C^\infty \left( \frac{Y_f \cup Y_b}{Y_f \cup Y_b} \right) \)

\[
- \int_{Y_f \cup Y_b} E \cdot \nabla \varphi_\Omega \, dx - \int_{Y_f \cup Y_b} \rho_\omega \varphi_\Omega \, dx - \int_{Y_f \cup Y_b} \rho_q \varphi_\Omega \, dx = 0, \tag{2.20a}
\]

\[
\int_{Y_f \cup Y_b} \frac{1}{\varepsilon_0} E \cdot \varphi_E \, dx - \int_{Y_f \cup Y_b} \Phi \left( \nabla \cdot \varphi_E \right) \, dx + \int_\Gamma \Phi \varphi_E \cdot \nu \, d\sigma = 0, \tag{2.20b}
\]

\[
\int_{Y_f \cup Y_b} \Phi \, dx = 0. \tag{2.20c}
\]
or for Equation 2.11 and all periodic \( \varphi, \Phi \in C^\infty(\overline{\Omega}) \), \( \varphi_E \in C^\infty(\overline{\Omega}) \)

\[
- \int_\Omega E \cdot \nabla \varphi \, d\mathbf{x} - \int_{\Gamma_s} \rho_{\text{el}}^{\Gamma_s} \varphi \, d\sigma - \int_\Omega \rho_{\text{el}} \varphi \, d\mathbf{x} = 0, \tag{2.21a}
\]

\[
\int_\Omega \frac{1}{\epsilon_0} E \cdot \varphi_E \, d\mathbf{x} - \int_\Omega \Phi (\nabla \cdot \varphi_E) \, d\mathbf{x} = 0, \tag{2.21b}
\]

\[
\int_\Omega \Phi \, d\mathbf{x} = 0. \tag{2.21c}
\]

In the following, we formulate the fully discrete system of equations. To do so, we drop the index \( r \) whenever no confusion is possible and note that the system of equations in (2.19) — discretized by (2.22) — has to be solved for every charged species while the system of equations in (2.20) or (2.21) — discretized by (2.23) or (2.24), respectively — has to be solved only once per time step. Moreover, we approximate the time derivative by the first order difference quotient to obtain an implicit Euler scheme. We proceed as follows:

Having defined two shape and contact regular families of geometrically conformal meshes (see Chapter 5 or [1, 9]) \( (\mathcal{T}_h)_{h>0} = (\mathcal{T}_h(\Omega))_{h>0} \) and \( \mathcal{T}_h(\Omega) \) with \( \mathcal{T}_h(\Omega)|_{\Omega_f \cup \Omega_b} = \mathcal{T}_h(\Omega_f \cup \Omega_b) = \mathcal{T}_h \),

their respective sets of faces \( \mathcal{F} = \mathcal{F}(\mathcal{T}_h) \) and \( \mathcal{F}_Y = \mathcal{F}(\mathcal{T}_h(\Omega)) \), and the broken polynomial spaces \( \mathbb{P}_{k}^{d}(\mathcal{T}_h), \mathbb{P}_{k}^{d-1}(\mathcal{F}|_{T}), \mathbb{P}_{k}^{d}(\mathcal{T}_h(\Omega)) \) (as in Chapter 5, [1, 9]), we can write the fully discrete system of equations by substituting \( \omega^\pm \leftarrow \omega^\pm_h, q \leftarrow q_h, \omega^{f,\pm} \leftarrow \omega^{f,\pm}_h, \Phi \leftarrow \Phi_h, \) and \( E \leftarrow E_h \), choosing discrete test and ansatz functions \( \varphi_i \in \mathbb{P}_k^{d}, \varphi_i \in \mathbb{P}_k^{d} \) that form bases of the respective polynomial spaces, and introducing appropriate inter-element fluxes.

In order to formulate the respective sets of equations, we additionally define \( \tau^n \) as the size of the \( n \)-th time-step, \( \mathcal{F}^{\pm}(\mathcal{K}) \) as the set of faces of \( \mathcal{K} \in \mathcal{T}_h \) whose elements are subsets of \( \Gamma, \mathcal{F}^{f}(\mathcal{K}) \) as its complement in \( \mathcal{F}(\mathcal{K}) \), and \( \mathcal{F}^{r}_{Y}(\mathcal{K}) \) as the set of faces of \( \mathcal{K} \) which also are boundaries of solid cells. Moreover, \( \| \cdot \| \) is a function’s interfacial average, \( \| \cdot \|_{t} \) is the jump (cf. Section 5.2.2), and \( (\cdot)^{\uparrow} \) is the upwind flux. For reasons of stability, the discrete evaluation of the upwind flux (i.e. the definition of the upwind direction) is done in every quadrature point and not integral-wise.

Thus — using the above notation — the following equations have to hold for every time-step \( n \in \{1, \ldots, N\} \), every basis function \( \varphi_i, \varphi_i, \) all \( \mathcal{K} \in \mathcal{T}_h \), and for all discrete functions \( \omega^{\pm,n}, \omega^{f,\pm,n}_h, q^n_h \), being linear combinations of their respective basis functions

\[
\int_{\mathcal{K}} (\omega^{\pm,n}_h - \omega^{\pm,n-1}_h) \varphi_i \, d\mathbf{x} - \tau^n \int_{\mathcal{K}} (q^n_h \pm C \omega^{\pm,n}_h E^n_h) \cdot \nabla \varphi_i \, d\mathbf{x}
\]
Chapter 2 Model for microaggregate development

\[ + \tau^n \sum_{F \in \mathcal{F}(K)} \int_F \left( \frac{\eta}{h_F} \omega_h^{\pm,n} \right) \cdot \nu \varphi_i \, d\sigma \]
\[ + \sum_{F \in \mathcal{F}(K)} \int_F \omega_h^{\pm,n} \varphi_i \, d\sigma - \tau^n \int_K \mathbf{R} \cdot \varphi_i \, d\sigma = 0, \quad (2.22a) \]
\[ \int_K D^{-1} q^n_h \cdot \varphi_i \, d\sigma = \int_K \omega_h^{\pm,n} (\nabla \cdot \varphi_i) \, d\sigma + \sum_{F \in \mathcal{F}(K)} \int_F \omega_h^{\pm,n} \varphi_i \cdot \nu \, d\sigma \]
\[ + \sum_{F \in \mathcal{F}(K)} \int_F \omega_h^{\pm,n} \varphi_i \cdot \nu \, d\sigma = 0, \quad (2.22b) \]
\[ \sum_{F \in \mathcal{F}(K)} \int_F \left( \omega_h^{\pm,n} - \omega_h^{\pm,n-1} \right) \varphi_i \, d\sigma \]
\[ + \sum_{F \in \mathcal{F}(K)} \left( -\tau k \int_F \mathbf{g} \left( \omega_h^{\pm,n} \right) \varphi_i \, d\sigma + \tau k \int_F \omega_h^{\pm,n} \varphi_i \, d\sigma \right) = 0, \quad (2.22c) \]
\[ \int_K \omega_h^{\pm,0} \varphi_i \, d\sigma - \int_K \omega_h^{\pm,0} \varphi_i \, d\sigma = 0. \quad (2.22d) \]

For the Poisson equation, we formulate that for every time-step \( n \in \{1, \ldots, N\} \), every basis function index \( i, i \), all \( K \in \mathcal{T}_h \), and for all discrete functions \( \Phi^n_h, E^n_h \) being linear combinations of their respective basis functions

\[ - \int_K E^n_h \cdot \nabla \varphi_i \, d\sigma + \sum_{F \in \mathcal{F}(K)} \int_F \left( \frac{\eta}{h_F} \Phi^n_h \right) \cdot \nu \varphi_i \, d\sigma \]
\[ - \int_K \rho_c \varphi_i \, d\sigma - \int_K \rho_c \varphi_i \, d\sigma = 0, \quad (2.23a) \]
\[ \int_K \frac{1}{\varepsilon_0} E^n_h \cdot \varphi_i \, d\sigma - \int_K \Phi^n_h (\nabla \cdot \varphi_i) \, d\sigma + \sum_{F \in \mathcal{F}(K)} \int_F \Phi^n_h \varphi_i \cdot \nu \, d\sigma \]
\[ + \sum_{F \in \mathcal{F}(K)} \int_F \Phi^n_h \varphi_i \cdot \nu \, d\sigma = 0, \quad (2.23b) \]
\[ \sum_{K \in \mathcal{T}_h} \int_K \Phi^n_h \, d\sigma = 0, \quad (2.23c) \]

or for every time-step \( n \in \{1, \ldots, N\} \), every basis function index \( i, i \), all \( K \in \mathcal{T}_h(Y) \), and for all discrete functions \( \Phi^n_h, E^n_h \) being linear combinations of their
respective basis functions

\[
- \int_{\mathcal{K}} E_h^n \cdot \nabla \varphi_i \, dx + \sum_{F \in \mathcal{T}_h(K)} \int_F \left( \frac{\|E_h^n\|}{h_F} + \frac{\| \Phi_h^n \|}{h_F} \right) \cdot \nu \varphi_i \, d\sigma \\
- \frac{1}{2} \sum_{F \in \mathcal{T}_h(Y(K))} \int_F \rho_e \, \varphi_i \, d\sigma - \int_{\mathcal{K}} \rho_e \, \varphi_i \, dx = 0, \quad (2.24a)
\]

\[
\int_{\mathcal{K}} \frac{1}{\varepsilon_0} E_h^n \cdot \varphi_i \, dx - \int_{\mathcal{K}} \Phi_h^n (\nabla \cdot \varphi_i) \, dx + \sum_{F \in \mathcal{T}_h(Y(K))} \int_F \| \Phi_h^n \| \varphi_i \cdot \nu \, d\sigma = 0, \quad (2.24b)
\]

\[
\sum_{\mathcal{K} \in \partial Y_h} \int_{\mathcal{K}} \Phi_h^n \, dx = 0. \quad (2.24c)
\]

The combination of (2.22) and (2.23) is a discretization of the NPP equation ((2.8) and (2.9)), while the combination of (2.22) and (2.24) is a discretization of the NPPSS equation ((2.8) and (2.11)). The latter one is used in the simulations.

### 2.C Appendix: Nomenclature for modeling

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha )</td>
<td>gluing agent</td>
</tr>
<tr>
<td>( \overline{\gamma} )</td>
<td>([L^{-1}/N(\text{T})^2]) proportional constant for stickiness</td>
</tr>
<tr>
<td>( \omega_0 )</td>
<td>([\text{N}/L^d]) concentration of r-th molecule</td>
</tr>
<tr>
<td>( c_{\text{Bac}} )</td>
<td>([\text{N}/L^d]) concentration of bacteria</td>
</tr>
<tr>
<td>( c_{\text{O}_2} )</td>
<td>([\text{N}/L^d]) concentration of oxygen</td>
</tr>
<tr>
<td>( \epsilon_0 )</td>
<td>([\text{F}^2/\text{T}^4/\text{M}^d]) dielectric permittivity</td>
</tr>
<tr>
<td>( \Gamma )</td>
<td>boundary of the solid phase</td>
</tr>
<tr>
<td>( \Gamma^s )</td>
<td>boundaries of all solid building units</td>
</tr>
<tr>
<td>( \Gamma_{\text{LG}} )</td>
<td>boundary between gas and liquid phases</td>
</tr>
<tr>
<td>( \hat{\gamma} )</td>
<td>([\text{N}^2]) proportional constant for attraction (or affinity)</td>
</tr>
<tr>
<td>( D )</td>
<td>([\text{L}^2/\text{T}]) effective diffusion tensor</td>
</tr>
<tr>
<td>( N )</td>
<td>number of cells in one spatial direction</td>
</tr>
<tr>
<td>( \nu )</td>
<td>([-]) outward unit normal of respective domain</td>
</tr>
<tr>
<td>( \nu_g )</td>
<td>([-]) outward unit normal of gas phase</td>
</tr>
<tr>
<td>( \omega_r )</td>
<td>([\text{N}/L^d]) concentration of r-th molecule only present in ( Y_f \cup Y_b )</td>
</tr>
<tr>
<td>( \omega^{\pm}_r )</td>
<td>([\text{N}/L^d]) concentration of r-th ion with ( \pm ) charge</td>
</tr>
<tr>
<td>( \otimes )</td>
<td>binary operator replacing cross product</td>
</tr>
<tr>
<td>( \partial Y )</td>
<td>periodic boundary of ( Y )</td>
</tr>
<tr>
<td>( \partial Y_i )</td>
<td>boundary of i-th cell</td>
</tr>
<tr>
<td>( \Phi )</td>
<td>([\text{M}L^2/\text{IT}^3]) electric potential</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>-------------</td>
<td>---------------------------------------------------------------------------</td>
</tr>
<tr>
<td>( \rho_e )</td>
<td>total charge density of volumetric species</td>
</tr>
<tr>
<td>( \rho^r_e )</td>
<td>total charge density of surface species</td>
</tr>
<tr>
<td>( \rho^s_e )</td>
<td>total charge density on solid blocks’ faces</td>
</tr>
<tr>
<td>( \theta )</td>
<td>porosity</td>
</tr>
<tr>
<td>( \theta_{\text{fluid}} )</td>
<td>fluid porosity</td>
</tr>
<tr>
<td>( \theta_{\text{liquid}} )</td>
<td>liquid porosity</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>proportional constant for breakup</td>
</tr>
<tr>
<td>( \tau )</td>
<td>time between updates of geometric structure</td>
</tr>
<tr>
<td>( \mathcal{D} )</td>
<td>scaling factor for specific surface</td>
</tr>
<tr>
<td>( \omega )</td>
<td>vector of concentrations of diffusing species</td>
</tr>
<tr>
<td>( \omega^r )</td>
<td>vector of concentrations of species on the surface</td>
</tr>
<tr>
<td>( E )</td>
<td>electric field</td>
</tr>
<tr>
<td>( e_j )</td>
<td>unit vector in ( j )-th spatial direction</td>
</tr>
<tr>
<td>( v )</td>
<td>velocity</td>
</tr>
<tr>
<td>( x_0 )</td>
<td>position of molecule/ion at time ( t_0 )</td>
</tr>
<tr>
<td>( A_i )</td>
<td>attraction (or affinity) of the ( i )-th neighboring cell</td>
</tr>
<tr>
<td>( c_{\alpha} )</td>
<td>concentration of gluing agent</td>
</tr>
<tr>
<td>( c_B )</td>
<td>concentration of biomass</td>
</tr>
<tr>
<td>( C_r )</td>
<td>electric drift constant</td>
</tr>
<tr>
<td>( c_{\text{B, min}} )</td>
<td>threshold value for transformation biom. ( \rightarrow ) bac.</td>
</tr>
<tr>
<td>( c_{\text{Bac, max}} )</td>
<td>threshold value for transformation bac. ( \rightarrow ) biom.</td>
</tr>
<tr>
<td>( c_{\text{up, ..., }} )</td>
<td>threshold value for agent growth</td>
</tr>
<tr>
<td>( c_{\text{up, ..., B}} )</td>
<td>threshold value for biomass growth</td>
</tr>
<tr>
<td>( D_r )</td>
<td>diffusivity of ( r )-th species</td>
</tr>
<tr>
<td>( D_{\text{O}_2, \beta} )</td>
<td>molecular diffusivity of oxygen in phase ( \beta )</td>
</tr>
<tr>
<td>( D_{\text{Bac, \beta}} )</td>
<td>molecular diffusivity of bacteria in phase ( \beta )</td>
</tr>
<tr>
<td>( f_{\text{decay}, a} )</td>
<td>decay rate for gluing agent</td>
</tr>
<tr>
<td>( f_{\text{up, O}_2, a} )</td>
<td>consumption rate of nutrient by gluing agent</td>
</tr>
<tr>
<td>( f_{\text{up, O}_2, B} )</td>
<td>consumption rate of nutrient by biomass</td>
</tr>
<tr>
<td>( f_{\text{up, O}_2, \text{Bac}} )</td>
<td>consumption rate of nutrient by bacteria</td>
</tr>
<tr>
<td>( f_{\text{gro. / dec.}} )</td>
<td>biomass growth and decay rate</td>
</tr>
<tr>
<td>( f_{\text{incr}, a} )</td>
<td>gluing agent increase rate</td>
</tr>
<tr>
<td>( f_{\text{incr, B}} )</td>
<td>biomass increase rate</td>
</tr>
<tr>
<td>( g )</td>
<td>Langmuir equilibrium isotherm</td>
</tr>
<tr>
<td>( G_r )</td>
<td>rate of heterogeneous reactions of the ( r )-th species</td>
</tr>
<tr>
<td>( H_{\text{O}_2}^{\text{L}} )</td>
<td>Henry’s law solubility constant for oxygen</td>
</tr>
<tr>
<td>( k )</td>
<td>rate constant</td>
</tr>
<tr>
<td>( R_r )</td>
<td>homogeneous rate for the ( r )-th diffusing species</td>
</tr>
<tr>
<td>( T )</td>
<td>end time</td>
</tr>
</tbody>
</table>

\[ \rho_e \], \[ \rho^r_e \], \[ \rho^s_e \], \[ \theta \], \[ \theta_{\text{fluid}} \], \[ \theta_{\text{liquid}} \], \[ \gamma \], \[ \tau \], \[ \omega \], \[ \omega^r \], \[ E \], \[ e_j \], \[ v \], \[ x_0 \], \[ A_i \], \[ c_{\alpha} \], \[ c_B \], \[ C_r \], \[ c_{\text{B, min}} \], \[ c_{\text{Bac, max}} \], \[ c_{\text{up, ..., }} \], \[ D_r \], \[ D_{\text{O}_2, \beta} \], \[ D_{\text{Bac, \beta}} \], \[ f_{\text{decay}, a} \], \[ f_{\text{up, O}_2, a} \], \[ f_{\text{up, O}_2, B} \], \[ f_{\text{up, O}_2, \text{Bac}} \], \[ f_{\text{gro. / dec.}} \], \[ f_{\text{incr}, a} \], \[ f_{\text{incr, B}} \], \[ g \], \[ G_r \], \[ H_{\text{O}_2}^{\text{L}} \], \[ k \], \[ R_r \], \[ T \]
## 2.C Nomenclature for modeling

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X(t; x_0)$</td>
<td>trajectory of a molecule/ion</td>
<td>39</td>
</tr>
<tr>
<td>$Y$</td>
<td>reference domain (quadratic (cubic), periodic)</td>
<td>32</td>
</tr>
<tr>
<td>$Y_i$</td>
<td>$i$-th grid cell</td>
<td>33</td>
</tr>
<tr>
<td>$Y_g$</td>
<td>$i$-th gas cell</td>
<td>32</td>
</tr>
<tr>
<td>$Y_f$</td>
<td>$j$-th fluid cell</td>
<td>32</td>
</tr>
<tr>
<td>$Y_b$</td>
<td>$k$-th bio cell</td>
<td>32</td>
</tr>
<tr>
<td>$Y_s$</td>
<td>$l$-th solid cell</td>
<td>32</td>
</tr>
<tr>
<td>$Y_b$</td>
<td>bio phase</td>
<td>33</td>
</tr>
<tr>
<td>$Y_f$</td>
<td>fluid phase</td>
<td>33</td>
</tr>
<tr>
<td>$Y_g$</td>
<td>gas phase</td>
<td>32</td>
</tr>
<tr>
<td>$Y_s$</td>
<td>solid phase</td>
<td>32</td>
</tr>
<tr>
<td>$z_r$</td>
<td>charge of $r$-th species</td>
<td>43</td>
</tr>
<tr>
<td>$b$</td>
<td>bio (cell)</td>
<td>33</td>
</tr>
<tr>
<td>CAM</td>
<td>cellular automaton method</td>
<td>29</td>
</tr>
<tr>
<td>f</td>
<td>fluid (cell)</td>
<td>33</td>
</tr>
<tr>
<td>g</td>
<td>gas (cell)</td>
<td>33</td>
</tr>
<tr>
<td>LDG</td>
<td>local discontinuous Galerkin</td>
<td>30</td>
</tr>
<tr>
<td>PDE</td>
<td>partial differential equation</td>
<td>30</td>
</tr>
<tr>
<td>s</td>
<td>solid (cell)</td>
<td>33</td>
</tr>
</tbody>
</table>
Chapter 3

Predicting the diffusion in porous media

Abstract of the chapter.  An accurate quantitative description of the diffusion coefficient in a porous medium is essential for predictive transport modeling (cf. the scenario in Section 2.4.9). Well-established relations such as proposed by Buckingham, Penman, and Millington–Quirk relate the scalar diffusion coefficient to the medium’s porosity. To capture the porous medium’s structure in more detail further models include fitting parameters, geometric, or shape factors. Some models additionally account for the tortuosity, e.g. via Archie’s law. A validation of such models has been carried out mainly via experiments relating the proposed description to a specific class of porous media (by means of parameter fitting).

Contrary to these approaches, upscaling methods directly enable calculating the full, potentially anisotropic, effective diffusion tensor without any fitting parameters. The only required input is the geometric information in terms of a representative elementary volume. To compute the diffusion–porosity relations, supplementary cell problems must be solved numerically, and their (flux) solutions must be integrated. This approach is applied to provide easy-to-use quantitative diffusion–porosity relations that are based on representative single grain, platy, blocky, prismatic soil structures, porous networks, or random porous media. As discretization discontinuous Galerkin methods on structured grids are used. To make the relations explicit, interpolation of the obtained data is carried out.

Furthermore, the obtained diffusion–porosity relations are compared with the well-established relations mentioned above and also with the well-known Voigt–Reiss and Hashin–Shtrikman bounds. We discuss the ranges of validity, provide explicit relations between diffusion and surface area, and comment on the role of a tortuosity–porosity relation.
Chapter 3  Predicting the diffusion in porous media

Outline of the chapter. In this chapter, we first review well-established relations such as given by Buckingham, Penman, and Millington–Quirk for a scalar diffusion coefficient in terms of porosity (cf. Section 3.2). Secondly, standard results from upscaling theory are stated (cf. Section 3.3.1). Here, integrating (flux) solutions of auxiliary cell problems allows calculating the full, potentially anisotropic, effective diffusion tensor. Then, the representative geometries under consideration are introduced, a literature overview is given, and the numeric solution and approximation strategies are briefly discussed in Section 3.4. We numerically evaluate the diffusion tensor in terms of porosity and total surface in Section 3.5. Additionally, explicit functional relations are derived via interpolation of the obtained data. In Section 3.5.1, we compare the outcome with the mentioned well-established relations and investigate the range of validity of these relations. In Section 3.5.2, the diffusion–total surface relation (see Section 2.2.4) is also investigated. Alternatively to explicit formulas or the computation of the effective diffusion tensor or its scalar representative, (sharp) bounds on the effective tensor are used including the arithmetic or harmonic mean, Voigt–Reiss bounds, or Hashin–Shtrikman bounds. We additionally evaluate and compare our results with respect to these bounds. Finally, relations between porosity and tortuosity and their impact on the diffusion coefficient are briefly discussed in Section 3.5.3.

Previously published articles. The content of the following chapter has already been published in


3.1 Introduction and motivation

Transport processes through porous media have a very long research history. Nevertheless, even the basic and most commonly used model equations and their parameters are still under investigation, cf. [75, 91, 92]. Thermal, and diffusive transport of chemical species are — in their simplest form — described by the following macroscopic/averaged transport equation:

\[ \partial_t \omega - \nabla \cdot (\mathbf{D} \nabla \omega) = f \]  (3.1)

with \( \omega \) describing the temperature or the species' concentration, and the coefficient \( \mathbf{D} \) representing effective thermal conductivity or effective diffusion for a chemical species, respectively. On the right-hand side, \( f \) includes sources and sinks.
3.2 Well-established functional relations for hydrodynamic parameters

The effective tensor $\mathbb{D}$ is the essential input to the transport model since it contains all the information that is specific to the considered porous medium. However, the full effective diffusion is very difficult to characterize in (natural) porous media — even if it is assumed that it is represented by a scalar $D_p$. Consequently, formulas in terms of simple features of the porous medium, e.g. the porosity, are frequently used (cf. the models by Buckingham, Penman, Marshall, and Millington–Quirk in (3.2)). Quintard states in [80] that porosity is the essential parameter for unconsolidated isotropic media. Consequently diffusion–porosity models often yield quite good approximations in such situations. The composition and structure of an arbitrary porous medium cannot, however, be accounted for by porosity variations only. Changes in particle distribution and grain shape and size — as described in Chapter 2 — modify tortuosity and connectivity of the pore-space and therefore the bulk response of the medium. To this end, parameters that are fitted to experimental data are included into further models. Power laws with fitting parameters such as proposed by Currie in [53] and further functional relations such as proposed for instance by Troeh et al. in [90] (cf. also (3.3)), have very good approximation properties when fitted to experimental data [90]. The main drawback of this remedy is that the model parameters often have no direct connection to the underlying porous medium structure, admit no physical interpretation, or are hard or even impossible to measure. In terms of applicability, explicit diffusion–porosity relations without any artificial parameters are most desirable, although in many practical applications one will not have good knowledge of pore-scale geometries and only have measurements of bulk porosity. This research contributes exactly to this point: Based on representative elementary volumes with representative soil structures, we calculate quantitative diffusion–porosity models that are easy to use (cf. Table 3.1). Note that another forward-looking approach is the rising field of digital rock simulations (see for instance [49, 55, 56]). Here, much more complex physical situations such as multiphase flow in real core samples are investigated. Our aim is, however, to obtain explicit formulas directly applicable in practice and also independent of very specific geometrical settings.

3.2 Well-established functional relations between hydrodynamic parameters and porosity

Finding suitable functional relations between porosity and effective tensor $\mathbb{D}$ or rather its scalar representative $D_p$ has been the topic of research for several decades. Well-known models for effective gas diffusion $D_p$ often assume a linear relation or power law in terms of porosity. The most commonly used relations nowadays are re-
viewed for instance in [62, 74, 91] and listed in (3.2). In these models, an exclusive dependence (i.e. without fitting parameters) of the effective gas diffusion $D_p$ on the gas diffusion coefficient in free air $D_0$ and the air filled porosity $\Psi$ is assumed:

$$\frac{D_p}{D_0} = \Psi^{2} \quad \text{Buckingham 1904 [50]}, \quad \frac{D_p}{D_0} = 0.66\Psi \quad \text{Penman 1940 [79]}, \quad \frac{D_p}{D_0} = \Psi^{3/2} \quad \text{Marshall 1959 [68]}, \quad \frac{D_p}{D_0} = \Psi^{4/3} \quad \text{Millington 1959 [71]}.$$

The above models have been derived by different approaches: The equations of Buckingham and Penman have been determined experimentally whereas the formulas of Marshall and Millington are based on theoretical calculations for a system of pores.

Due to the general complexity of porous media, the same porosities may induce different effective tensors (see also Section 3.5.1 and Section 2.4.3 for a numerical illustration). Hence, there is already numerous research additionally taking geometric/structural information into account, for instance via shape factors, the total surface, the tortuosity or further (measurable) parameters. Models including fitting parameters based on empirical data are, amongst others, given by the following relations:

$$\frac{D_p}{D_0} = \phi \Psi^{\xi} \quad \text{Currie 1960 [53]} \quad \text{and} \quad \frac{D_p}{D_0} = \left(\frac{\Psi-u}{1-u}\right)^{v} \quad \text{Troeh 1982 [90]} \quad (3.3)$$

A drawback to functional relations of the form $\phi \Psi^{\xi}$ with parameters $\phi$, $\xi$ is that diffusivity degenerates only for $\Psi = 0$. This model assumption is a very strong restriction and not reasonable for most geometric settings, cf. investigations in Section 3.5.1. Since the pore space may be disconnected if single grains touch each other, the diffusivity may already degenerate for positive porosities. Furthermore, the physical requirement $D_p(\Psi) = D_0$ for $\Psi = 1$ immediately leads to $\phi = 1$ and $\xi$ remains the only fitting parameter. However, fitting the two-parameter model to experimental data yields reasonable approximation quality, since the unphysicality in that model is then balanced with possible choices of $\phi \neq 1$. In [90] the following improvement was made to the model: $\left(\frac{\Psi-u}{1-u}\right)^{v}$ with two parameters $u, v$. In this model, the condition $D_p(\Psi) = D_0$ for $\Psi = 1$ is naturally satisfied. Moreover, the model accounts for the degeneration of the diffusion coefficient even for positive porosities. More precisely $D_p(\Psi) = 0$ for all $\Psi \leq u$.

For unsaturated media the situation becomes more complex and the related models become more involved, Millington and Quirk propose the following relations in terms of the soil total porosity $\Theta$ (opposed to the air filled porosity $\Psi$; for a definition of $\Theta$ consider Section 2.2.4), cf. review in [75]:

$$\frac{D_p}{D_0} = \frac{\Psi^2}{\Theta^{2/3}} \quad \text{and} \quad \frac{D_p}{D_0} = \frac{\Psi^{10/3}}{\Theta^{2}}, \quad \text{which both reduce to } \Psi^{4/3} \text{ for } \Psi = \Theta.$$
to 11 and the air filled porosity $\Psi_{100}$ at -100 cm $H_2O$ of soil water matrix potential into the models to obtain the so-called Buckingham–Burdine–Campbell (BBC) model $\frac{D_p}{D_0} = \theta^2 \left( \frac{\Psi}{\theta} \right)^{2+3b}$ and $\frac{D_p}{D_0} = (2\Psi_{100}^3 + 0.04\Psi_{100}) \left( \frac{\Psi}{\theta} \right)^{2+3b}$, respectively. Finally, Olesen et al. included the volumetric soil surface area $SA_{vol}$ into their model to obtain $\frac{D_p}{D_0} = 1.1\Psi (\Psi - 0.039SA_{vol}^{0.52})$, cf. the review in [74].

Beyond that, there is extensive work of Hunt et al. (cf. [64] for a review) who apply percolation theory to many porous media problems including diffusion and the classic book [89] containing a lot of valuable information.

Along these lines, there is an unmanageable number of formulas for the scalar diffusion coefficient depending not only on porosity, but also on numerous (artificial) parameters and physical variables. However, in terms of applicability low parameter models being particularly independent of hard to measure input are most desirable. Moreover, many of the cited models are derived from fitting to data and often are only valid in a restricted range of porosity. Additionally, the fundamental drawback of all models listed in (3.2) and their modifications or extensions is: They refer to scalar coefficients rather than to the full, potentially anisotropic, effective diffusion tensor. This simplification is only verified for isotropic porous media; compare also the discussion in Section 3.3.2 and the numerical illustrations in Section 3.5.1. The approach presented in the following contrarily enables computing the full effective diffusion tensor for a prescribed representative geometry without any further fitting parameters.

### 3.3 Mathematical models and bounds

If the underlying geometry of a representative elementary volume $Y$ is prescribed, cf. Figure 3.1 and Figure 3.2, certain mathematical theories are available that make it possible to calculate the full, potentially anisotropic, tensor $D$. Starting from mathematical models at the pore-scale, an averaging procedure is performed to derive effective models. For the transport equation, e.g. a diffusion equation with molecular/free diffusion $D_0$ is the starting point. Volume averaging [98], thermodynamically constrained averaging theory (TCAT) [59], two-scale asymptotic expansion [48] or, mathematically more rigorous, two-scale convergence [45, 76] may be applied to these equations. As a result of the averaging procedure, the averaged transport equation as introduced in Section 3.1 can be derived.

In order to derive an effective model approximating the original problem (3.1) via formal two-scale asymptotic expansion we assume that an unknown $\omega_\varepsilon$ may be represented with respect to the scale parameter $\varepsilon > 0$, i.e.

$$
\omega_\varepsilon(x, t) = \omega(x, x/\varepsilon, t) + \varepsilon \omega^1(x, x/\varepsilon, t) + \varepsilon^2 \omega^2(x, x/\varepsilon, t) + \ldots .
$$
with sufficiently smooth functions $\omega, \omega^k, k \in \mathbb{N}$ depending on the two spatial variables $x$ ("macroscopic") and $y := x/\epsilon$ ("microscopic"). With respect to $y$ these functions are assumed to be periodic. Then, the effective tensor $\mathbb{D}$ is given explicitly as the integral over (flux) solutions of auxiliary cell problems which are defined for a representative elementary volume, cf. (3.4) below.

In Section 3.3.1, the effective tensor is defined in (3.4) and the auxiliary cell problems are given in (3.5). Moreover, special cases, in which the general form of effective tensors simplifies or sharp bounds may be obtained, are emphasized in Section 3.3.2.

### 3.3.1 Standard upscaling results

In the following, the porosity $\theta = \frac{|Y_f|}{|Y|}$ is defined as the volume of the connected, sufficiently smooth pore space $Y_f$ (where diffusion takes place) with respect to the total volume of the $n$-dimensional representative elementary volume $Y = [0,1]^n$, $n = 2, 3$. Hence, in the context of Chapter 2 no gas and no bio phases occur. The solid (where no diffusion takes place) is given by $Y_s := Y \setminus Y_f$. Let the non-negative function $D : Y \rightarrow \mathbb{R}$ describe the diffusivity within $Y$. Further, according to [61] we hypothesize that for the diffusion tensor $D$, it holds

$$D_{ij} := \frac{1}{|Y|} \int_{Y_f} D(y) (\partial_y \zeta_j + \delta_{ij}) \, dy$$

(3.4)

with supplementary cell problems for $\zeta_j, j = 1, \ldots, n$

$$\begin{cases}
-\nabla_y \cdot (\nabla_y \zeta_j + e_j) = 0 & \text{in } Y_f, \\
(\nabla_y \zeta_j + e_j) \cdot \nu = 0 & \text{on } \partial Y_s, \\
\zeta_j \text{ is periodic in } y \text{ and has vanishing mean.}
\end{cases}$$

(3.5)

Hereby, $\nu$ denotes the unit outward normal, $e_j$ the unit vector in direction $j$, and $\delta_{ij}$ the Kronecker delta.

A functional relation between effective tensor $\mathbb{D}$ and porosity is derived from this theory if different $Y_s$ (leading to different porosities) are investigated. In Section 3.4, this procedure is described in more detail for representative soil structures.

### 3.3.2 Special cases and analytical bounds

**Isotropic media.** For isotropic media, the effective tensor reduces to a scalar $D = D_p \mathbb{E}$ with unity matrix $\mathbb{E}$. Such settings are numerically evaluated and illustrated in Section 3.5.1, Figure 3.3 and Figure 3.4.
Layered medium. As described in [61, Chap. 1, Prop. 3.3], for an \( n \)-dimensional, layered medium, characterized by \( D(y) = D(y_1, \ldots, y_n) = \bar{D}(y_n) \), the cell problems’ solutions of (3.5) may be calculated explicitly:

\[
\zeta_n = \int_0^{y_n} \frac{1}{\bar{D}(\eta)} \, d\eta - y_n \quad \text{and} \quad \zeta_j = 0 \quad \text{for} \ j \neq n,
\]

and the effective tensor according to (3.4) is given by

\[
\mathbb{D}_{nn} = \bar{D} \left( \int_0^1 \frac{1}{\bar{D}(\eta)} \, d\eta \right)^{-1} \quad \text{and} \quad \mathbb{D}_{ij} = \bar{D} \delta_{ij} = \left( \int_0^1 \bar{D}(\eta) \, d\eta \right) \delta_{ij}
\]  

(3.6)

for \( i \neq n \) and \( j \neq n \). These are the harmonic mean \( \bar{D} \) and the arithmetic mean \( \bar{D} \) vertical and parallel to the layers, respectively.

If the medium has for instance \( k \) layers of equal thickness \( 1/k \) and the diffusion is constant and equal to \( D_\ell, \ell = 1, 2, \ldots, k \) in each of the \( k \) layers, we have for \( i \neq n \) and \( j \neq n \)

\[
\mathbb{D}_{nn} = \bar{D} = \left( \int_0^1 \frac{1}{\bar{D}(\eta)} \, d\eta \right)^{-1} \quad \text{and} \quad \mathbb{D}_{ij} = \bar{D} \delta_{ij} = \frac{1}{k} \left( \sum_{\ell=1}^k D_\ell \right) \delta_{ij}.
\]

As a second example, we consider a two-dimensional porous medium with porosity \( \theta \) consisting of a system of horizontal tubes with constant diffusivity \( D(y) = D_0 \) and impermeable porous matrix. Then, it holds

\[ D_{22} = \bar{D} = 0 \quad \text{and} \quad D_{ij} = \bar{D} \delta_{ij} = \theta D_0 \delta_{ij} \quad \text{for} \ i \neq 2 \ \vee j \neq 2. \]

Hence, in this setting, the upscaling approach states that diffusivity depends linearly on porosity for the non-degenerating eigenvalue. This perfectly matches the model given by Penman in [79], cf. Equation (3.2), with the exception to the prefactor. For an interpretation of the prefactor in terms of tortuosity, please refer to the discussion in Section 3.5.3.

Bounds. Unfortunately, in the most cases (including even isotropic ones) it is not possible to calculate the homogenized parameters via (3.4) analytically due to the periodic boundary conditions. However, the Voigt–Reiss inequality asserts that the harmonic or arithmetic mean provide lower or upper bounds, respectively, for the effective diffusion tensor defined in (3.4), cf. [66, Sec. 1.6]: Assuming that the diffusivity \( D(y) \) at the pore scale is periodic with respect to the representative
elementary volume \( Y := [0,1]^n \), the following estimate holds (in the sense of eigenvalues):

\[
\left( \int_Y \frac{1}{D(\eta)} \, d\eta \right)^{-1} \leq \mathbb{D} \leq \int_Y D(\eta) \, d\eta.
\] (3.7)

Let us for instance consider a two-dimensional isotropic porous medium with porosity \( \theta \) and diffusion tensor \( D(y) \), where \( D(y) = D_0 > 0 \) within the pores and \( D(y) = 0 \) within the impermeable porous matrix. To apply the Voigt–Reiss inequality, we approximate \( D(y) \) by \( D_c(y) \) with \( D_c(y) = D_0 \) in the pore space and \( D_c(y) = \epsilon > 0 \) within the porous matrix. Then (3.7) yields

\[
D_p \leq \theta D_0 + (1 - \theta) \epsilon, \quad \text{i.e. we obtain} \quad \frac{D_0}{D_0} \in [0, \theta] \quad \text{for} \quad \epsilon \searrow 0.
\]

This is also evident from the simulations in Section 3.5.1, Figure 3.3 and Figure 3.4 since all curves are localized below the angular bisector of the first quadrant.

As a second example we consider layered media as discussed in the previous section. In this situation, the Voigt–Reiss bounds are sharp, see also [66, Sec. 1.2, (1.25)], and the bounds can be interpreted as a generalization of the layered media situation to arbitrary underlying geometries.

The bounds provided by the Voigt–Reiss inequality are often not sharp enough. For isotropic two-phase materials the best bounds that do not take into account particular geometric properties are given by the so-called Hashin–Shtrikman bounds: Let \( D(y) = D_1 \chi(y) + D_2 (1 - \chi(y)) \) be the scalar diffusivity of an isotropic two-phase material, where \( D_1, D_2 \) are the two values of diffusivity and \( \chi \) is the characteristic function of \( \{ y \in [0,1]^n : D(y) = D_1 \} \). If \( D_1 < D_2 \) and \( \theta = 1 - \int_Y \chi(\eta) \, d\eta \) denotes the respective volume fraction of the material with diffusivity \( D_2 \), we have

\[
D_1 \left( 1 + \frac{n \theta (D_2 - D_1)}{n D_1 + (1 - \theta) (D_2 - D_1)} \right) \leq D_p \leq D_2 \left( 1 - \frac{n (1 - \theta) (D_2 - D_1)}{n D_1 + \theta (D_2 - D_1)} \right),
\]

cf. [66, Sec. 6.1, (6.8)]. In the case of porous media, we assume that one material representing the porous matrix is impermeable, i.e. \( D_1 = 0 \) and \( D_2 = D_0 \). Then \( \theta \) describes the porosity and the above inequality yields \( \frac{D_p}{D_0} \in [0, \frac{n-1}{n-\theta}] \). This estimate yields a very good approximation, cf. the simulations in Section 3.5.1 where the excluded area is visualized in gray in Figure 3.3 and Figure 3.4. Chang [51] also obtained the upper bound \( \frac{1}{2-\theta} \) by analytically solving a modified two-dimensional cell problem (3.5) (\( Y \) and \( Y_s \) are approximated by concentric circles). This approximative result was validated numerically and extended to anisotropic, ellipsoidal unit cells, cf. [78]. In three dimensions the upper Hashin–Shtrikman bound \( \frac{2}{3-\theta} \) was already given by Maxwell in [69] and De Vries in [54] for the electric conductivity of media containing spherical inclusions.

In particular, for small porosities the three-dimensional Hashin–Shtrikman bound \( \frac{2}{3-\theta} \) is approximated linearly by \( \frac{2}{3} \theta \approx 0.66 \theta \). Thus, the model of Penman (3.2) may be interpreted as the Taylor expansion in zero of the upper
Hashin–Shtrikman bound up to first order. Hence, the model given by Penman provides a reasonable relation for small porosities and non-degenerating diffusion.

Moreover, in [97] the bound \( \frac{2}{2 - \ln(\theta)} \theta \) is deduced by investigating statistical specifications of the porous medium. More precisely, the derivation of this bound is based on randomly overlapping three-dimensional spheres. In the case of overlapping spheres, i.e. for porosities \( \theta \leq 1 - \frac{\pi}{6} \approx 47.6\% \) the stated bound is an improvement to the upper bound given by Hashin–Shtrikman, cf. illustration of bounds in Figure 3.4 and Figure 3.5.

### 3.4 Setting and numerical methods

#### Figure 3.1: Representative elementary volumes in 2D: Square, circle, rectangles of type 1 with different but fixed height, rectangle of type 2, ellipse, crosses of types 1 and 2, octagon, hexagon, and random geometry.

#### Figure 3.2: Representative elementary volume in 3D: Cube, sphere, 3D cross, hexagonal prism, and random.

Assumptions must be made for the microstructure, which is hard to access, to apply the mathematical theory that has been introduced in Section 3.3.1. Representatives for single grain, platy, blocky, prismatic soil structures, porous networks, or random porous media are used in the representative elementary volumes, cf. Figure 3.1 and Figure 3.2. Such geometries often serve as model systems for hypothesis testing. Idealized porous media are, amongst others, frequently used to represent soil [77] due to its tremendous complexity. 2D representatives, e.g. prototypes with rough (potentially structured) planar surfaces, 3D transparent model systems consisting of silica glass beads which facilitate imaging, or devices from 3D printing techniques creating sophisticated model systems with
controlled surface properties and topologies are used [60]. The chosen model systems also mimic artificial model systems that directly arise in technical applications. Examples are microfluidic systems such as 1D analogues of porous media [58] or microwells which allow the precise geometric positing or trapping of cells for cultivation or further studies. The cells may for instance be comprised of honeycomb structures [63]; recently, 3D porous cubes which facilitate oxygen diffusion have also been investigated [81].

To derive diffusion–porosity relations, straight or perturbed channels are often considered. These may basically serve as 1D representatives for porous media, cf. [58]. In [47], a perturbed straight channel is considered in the representative elementary volume, and the cell problems (3.5) and the effective tensor (3.4) are evaluated. In [84] the same setting is considered and interpreted in the context of tortuosity.

Kim et al. use model systems of 2D rectangles with different aspect ratios in regular packings to compare the results with their experimental data for glass spheres, mica particle and mylar disks in [67]. Quintard investigates the same situation but uses cylinders with different orientation as better representatives for mylar disks in 3D to calculate the effective anisotropic diffusion tensor, cf. [80]. Additionally, different isotropic sphere packings are discussed in [80]. In [57], effective diffusion and tortuosity are related for bentonite with laminar montmorillonite structures (layered porous medium). Thereby, a comparison of straight and winding paths and their combination is considered. As a model system 2D stacks of rectangles potentially forming a cross-like structure are used. In Smith [87] a combination of rectangles with different orientations is used to represent platy clays. In their study the role of ion exclusion for the actual diffusion coefficient is investigated. In [85] rectangular and triangular geometries are considered and the effective tensor (3.4) over the porosity is evaluated. Similarly, in [96] a circular geometry is considered. In the context of thermal conductivity, Ijioma et al. [65] consider elliptic inclusions of different orientations. In [46], an even more complex situation is considered: In an anisotropic rectangular geometry, the permeability and electro-diffusion tensors over porosity are calculated, which finally lead to a non-monotonic functional relation for the cations. Similarly, in [82], different interaction potentials related to van der Waals interaction rather than electric ones are considered and effective permeability and diffusion tensors over porosity are evaluated. In [3] a more complex geometric situation, namely diffusion tensors based on randomly generated and consolidating geometries, is investigated. Moreover, the impact of homogeneous [93] and heterogeneous [94] reactions on the effective diffusion is investigated for cubic inclusions in two and three dimensions using volume averaging techniques. In the same setting, Valdes et al. [95] interpret their numerical
and analytical findings in the context of tortuosity. Ochoa et al. [78] extend the results by Chang [51] by considering ellipsoidal inclusions and compare their results, amongst others, with experimental data and the findings of Kim and Quintard [67, 80]. Finally, Miller et al. [70] compute the effective diffusion for 3D spherical inclusions and fiber bundles applying TCAT and [88] use finite element simulations to evaluate diffusion tensors in the presence of an advective field.

In agreement with the literature, the geometries depicted in Figure 3.1 and Figure 3.2 may serve as reasonable model systems for different soil structures. The circle/sphere and ellipse represent single grain or granular soils such as sandy soils or artificial model systems consisting of glass beads. In case that the circle or sphere touches the boundary of the representative elementary cell a primitive cubic packing is obtained. Rectangles on the other hand have widely been used to represent platy structures. In case that rectangles touch the boundary of the elementary volume, a system of tubes is obtained. Likewise, cubes represent blocky soil, and cuboids represent prismatic soils respectively. Similarly, the hexagonal and octagonal structures depicted in Figure 3.1 and Figure 3.2 may represent platy or prismatic soils. Quintard already states in [80] that two-dimensional model systems fail if unconsolidated anisotropic systems are considered. Consequently, 3D model systems are included into this research, cf. Figure 3.2. Along that line, we additionally investigate 3D porous networks and random porous media that better mimic general natural porous media. To create random domains of different porosities the C++ functions void std::srand(unsigned int) and int std::rand(void) have been used to determine whether a cell / voxel is fluid or solid. Hence, the solid and fluid cells / voxels are uniformly distributed in each spatial direction.

To obtain a diffusion–porosity relation for large ranges of porosities (opposed to quite small ranges accessible in experiments) based on the prescribed geometries, the evolution of the porous matrix represented by the white/red inclusions in Figure 3.1 and Figure 3.2 is prescribed in such a way that its general shape is maintained. For the square/cube and circle/sphere the evolution is uniform in radial direction and in direction of the axis, respectively. For rectangles of different thickness uniform evolution in width is considered (type 1), i.e., starting with a rectangle as shown in the third picture of Figure 3.1 growth leads to a rectangle as in the fourth picture of Figure 3.1. Moreover, rectangles of type 2 and the ellipse evolve uniformly in width and also in height (c.f. growth from a rectangle as depicted in the third picture of Figure 3.1 leading to a rectangle as depicted in the fifth picture, for example). For the cross two different evolutions are taken into account: First a pure lengthening of the cross arms along their axes (type 1) and second an additional thickening of the cross arms while lengthening.
In three spatial dimensions, the crosses form a network, i.e., the arms of the crosses meet one another and their evolution is due to the thickening of their arms. Likewise, the random geometries as depicted in Figure 3.1 are evolving as described in Chapter 2. The algorithm for such a consolidation is discussed in the context of soil microaggregates in Section 2.2.3 (here applied in a simplified version with $\gamma = 0$ in (8) of [3]) and is based on the ideas in [52].

For the investigations made in the cited references only graphical evaluations of the diffusion–porosity relation are given. Only in [96] interpolation of the obtained data has been done to provide easy to use power laws for diffusion and also permeability. We contribute exactly to this point and provide quantitative diffusion–porosity relations based only on the prescribed representative geometry, cf. Table 3.1. Along the same lines, relations with respect to the total surface are provided, cf. Table 3.2. To this end, first the solutions to the auxiliary cell problems (3.5) and then, the effective diffusion tensor defined in (3.4) are computed. As discretization method for the underlying partial differential equations the local discontinuous Galerkin scheme is used on structured grids within the software toolbox M++ [43]. Discontinuous Galerkin methods generally use element-wise polynomial but globally discontinuous ansatz functions. The local discontinuous Galerkin method uses a mixed formulation where second (or higher) order equations are replaced with a system of first order equations by introducing auxiliary flux variables. This is advantageous since it yields a direct representation of $V_y \zeta_j$ in (3.4), (3.5). For an analysis and detailed description of the used method please refer to Chapter 5. Moreover, this method allows to tune the discretization to either minimize numerical diffusion or further increase stability by means of penalty terms [1]. Additionally, I experienced that for low porosities and complex geometries mixed finite elements did not yield positive semi-definite tensors, while the discontinuous Galerkin method still gave reasonable tensors. For “easy” geometries, on the other hand, both methods’ tensors were extremely similar. The meshes for the non-random geometries in 2D comprise $128 \times 128$ elements. Those in three dimensions comprise $64^3$ elements. All meshes for random geometries consist of 32 squares / voxels in each spatial dimension.

To make our investigations quantitatively, we determine suitable best approximating functions. For the diffusion–porosity relation, the same functional form of $\frac{D_p}{D_0} = \left(\frac{\theta - \hat{\theta}}{1 - \hat{\theta}}\right)^b$ with parameters $b, \hat{\theta}$ as in the model proposed by Troeh in (3.3) is considered. The results are summarized in Section 3.5.1, see Table 3.1. Contrarily to Troeh, the parameters are not determined by fitting to experimental data but by analyzing the underlying geometry and approximating the numerical data obtained for the diffusion coefficient. It obviously holds $D_p = D_0$ for
\( \theta = 1 \) and the parameter \( \widehat{\theta} \) describes the largest porosity such that the diffusion coefficient \textit{degenerates}, i.e. \( D_p(\theta) = 0 \) for \( \theta \leq \widehat{\theta} \). The parameter \( \widehat{\theta} \) depends significantly on the underlying geometry and (up to the random geometry) can be calculated analytically. In this sense, we obtain a one-parameter model with parameter \( b \) which finally controls the shape of the \( \theta-D_p \) graph and cannot be determined analytically. Instead, we use the obtained numerical data for the diffusion tensors based on porosity variations to determine the parameter \( b \). In doing so, we minimize the error via the MATLAB\textsuperscript{2016a}\textsuperscript{1}-function \texttt{nlinfit}.

The main advantage of our approach compared to the investigations in \textit{Troeh} is that rather than fitting experimental data the underlying geometry explicitly determines the parameter \( \widehat{\theta} \) and indirectly also determines the parameter \( b \), so to speak.

In the second fitting approach we quantitatively investigate the relation between diffusion and \textit{total surface} \( \sigma \). The numerical data for the diffusion tensor is approximated by a function of the form \( 1 - \left( \frac{\sigma}{\widehat{\sigma}} \right)^b \), where \( \widehat{\sigma} \) is inversely to \( \widehat{\theta} \) the smallest surface area such that the diffusivity degenerates (i.e. \( D_p(\sigma) = 0 \))

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.3}
\caption{Scalar representative \( \frac{D_p}{D_0} \) over porosity for isotropic geometries in 2D: Square, circle, cross (type 1 and 2), and octagon; Hashin–Shtrikman bound \( \frac{\theta}{\theta^2} \) (exclusion of gray area); functional relations \( \theta^{3/2} \) (Marshall 1959) and \( \theta^2 \) (Buckingham 1904).}
\end{figure}
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for $\sigma \geq \widehat{\sigma}$) and may again be determined analytically from the underlying geometry. The parameter $b$ is again determined by minimizing the error via the MATLAB2016a\-function $\text{nlinfit}$, see Table 3.2 in Section 3.5.2.

In both cases, $\text{nlinfit}$ was used with the options

\begin{verbatim}
 opts = statset('nlinfit'); opts.RobustWgtFun = 'bisquare'.
\end{verbatim}

A detailed description of this method can be found on https://de.mathworks.com/help/stats/nlinfit.html (2017-12-05, 2PM).

3.5 Evaluation

In this section, we evaluate the outcome of our numerical simulations qualitatively and also quantitatively. We first discuss the diffusion–porosity relation and draw conclusions related to well established relations and bounds as discussed in Section 3.2 and Section 3.3.2. Then, analogue results related to the total surface are discussed and the role of tortuosity is briefly outlined.

3.5.1 Evaluation of effective tensors over porosity

The diffusion–porosity relation is investigated first. For soils, the range of porosity lies between 30% and 70% [77]. Since idealized porous media are often considered to represent soil porosity ranges related to sphere packings, they are of particular interest. Uniform packed spheres have porosities between 26% and 48%. The porosity for densest packings range from 26% to 32% for cubic body centered packings. Random packings have porosity ranges between 30% and 35% and yield good approximations for sandy soils. Although polydisperse sands could theoretically fall to porosities below 26%, this is improbable. Instead porosities of 30%–35% are obtainable [77]. However, porous rocks such as sandstone may have very low porosities (<30%) and peat soils contrarily have porosities up to 80%–90% [77]. In this sense the whole range of porosities is relevant and investigated within this research. Experiments contrarily focus mainly on porosities below 60% and only on small variations of 20%–30%, cf. the data brought together in [90]. For such small ranges, power laws or even linear models may yield quite accurate approximation properties. However, outside these ranges the obtained models may be quite inaccurate or inherit even unphysical properties, consider for instance the situation of large porosities in the linear

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Figure 3.4: Scalar representative $\frac{D_p}{D_0}$ over porosity for isotropic geometries in 3D: Cube, sphere, and Hashin–Shtrikman bound $\frac{\theta}{\bar{\theta}}$ (exclusion of gray area); functional relations $\theta^{4/3}$ (Millington–Quirk 1961), $\theta^{3/2}$ (Marshall 1959), and $\theta^2$ (Buckingham 1904).

model $0.66\theta$ of Penman or the power law $2.8\theta^3$ given by Papendick/Campbell or the fittings of experimental data to power laws provided and illustrated in [90]. One main advantage of the presented approach is that the full range of porosity $\theta \in [0\%, 100\%]$ may be investigated to obtain reasonable quantitative relations in the whole domain of definition. Note that for small porosities other discretization methods than the local discontinuous Galerkin method may fail due to stability issues. Moreover, computations tend to be more time-consuming since the conditions of the discretization matrices get larger. This results in the need of more iterations for solving the linear system of equations using BiCGStab.

The results are illustrated as follows: The scalar representation $\frac{D_p}{D_0}$ or eigenvalues of $\frac{D}{D_0}$ over porosity are depicted for isotropic geometries in Figure 3.3 and Figure 3.4 and for anisotropic geometries in Figure 3.6. Likewise, the results for random geometries are illustrated in Figure 3.7.

Note that significantly different values are obtained for effective diffusion tensors for the same porosity values, but different underlying geometries. In this sense it is evident that the underlying geometry, i.e. shape and composition, play an essential role for the diffusion–porosity relation. It is also evident from Figure 3.3
Figure 3.5: Scalar representative $\frac{D_p}{D_0}$ over porosity $\theta \in [0\%, 50\%]$ for isotropic geometry sphere in 3D, our approximated polynomial from Table 3.1, and the upper bound of Weissberg $\frac{2\theta}{2-\ln(\theta)}\theta$ (exclusion of gray area); functional relations $\theta^{4/3}$ (Millington–Quirk 1961), and $\theta^{3/2}$ (Marshall 1959).

(e.g. cross) and Figure 3.6 (rectangle type 1) that the diffusion tensor may also degenerate for non-vanishing porosities both in the isotropic and anisotropic cases. In such cases the drop to zero may even occur for comparable high values of the porosity. Troeh [90] already accounted for such degenerations with the shift factor $u$, cf. (3.3). For the situation of glass beads Troeh fitted his parameters $u, v$ in (3.3) to the experimental data of Penman, Currie, and Millington & Quirk and obtained the following parameters ranges: $u \in [0\%, 5\%]$ and $v \in [1.3, 1.4]$. Fitting the numerical data for a spherical geometry to the same functional form $\frac{D_p}{D_0} = \left(\frac{\theta - \hat{\theta}}{1 - \hat{\theta}}\right)^b$ yields $\hat{\theta} \approx 3.49\%$ and $b \approx 1.3519$, cf. Table 3.1. Since glass beads are very well represented by three-dimensional spheres, a good match of the fitting parameters was obtained.

It must be recognized that a regular simple sphere packing can be obtained in the case of touching spheres in 2D and in 3D leading to a porosity value of $1 - \frac{\pi}{4} \approx 21.5\%$ and $1 - \frac{\pi}{6} \approx 47.6\%$, respectively. In contrast to 2D where touching circles lead to degenerating diffusivity, the diffusion coefficient does not degenerate even for overlapping spheres in three dimensions, more precisely
Figure 3.6: Left: Eigenvalues of $\frac{D}{D_0}$ over porosity for anisotropic geometries in 2D: Rectangle type 1 (varying width but fixed height), rectangle type 2, and ellipse (varying width and height). Right: Eigenvalues of $\frac{D}{D_0}$ over porosity for (an-)isotropic geometries in 3D: Cross 3D (with varying width) and hexagonal prism.

Figure 3.7: Eigenvalues of $\frac{D}{D_0}$ over porosity for random geometries in 2D (left) and 3D (right).

for the range $\theta \in (1 + \frac{\sqrt{8}}{3} \pi - \frac{5}{4} \pi, 1 - \frac{7}{9} \pi)$. Since the upper bound by Weissberg [97] is derived via randomly overlapping spheres, it yields a very good upper bound for the diffusion coefficient in this porosity range, cf. Figure 3.5. The quite simple functional relation $\theta^{3/2}$ by Marshall almost perfectly matches the numerical data obtained from upscaling theory in the case of three-dimensional spherical geometries over the complete porosity range, cf. Figure 3.4. However, the fitting to $(\frac{\theta - \tilde{\theta}}{1 - \tilde{\theta}})^b$ with parameters $\tilde{\theta} \approx 3.49\%$ and $b \approx 1.3519$ yields an even better approximation, cf. Figure 3.5.
### Table 3.1: Quantitative relations of $D_p/D_0$ on porosity. Note that the ansatz functions are $D_p/D_0 = 0$ for $\theta \leq \tilde{\theta}$ and $D_p/D_0 = \left(\frac{\theta - \tilde{\theta}}{1 - \tilde{\theta}}\right)^b$ otherwise, where $\tilde{\theta}$ and $b$ are given in the above table. Note that the coefficients of random geometries are given in intervals (evaluated for 100 different random calculations) for the smallest eigenvalue.

<table>
<thead>
<tr>
<th>Geometric Shape</th>
<th>$\tilde{\theta}$</th>
<th>$b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Square</td>
<td>$0%$</td>
<td>$1.7301$</td>
</tr>
<tr>
<td>Circle</td>
<td>$1 - \frac{\pi}{4} \approx 21.46%$</td>
<td>$1.1734$</td>
</tr>
<tr>
<td>Cross (type 1)</td>
<td>$64%$</td>
<td>$0.6374$</td>
</tr>
<tr>
<td>Cross (type 2)</td>
<td>$4%$</td>
<td>$1.6071$</td>
</tr>
<tr>
<td>Octagon 2D</td>
<td>$12.5%$</td>
<td>$1.3945$</td>
</tr>
<tr>
<td>Cube 3D</td>
<td>$0%$</td>
<td>$1.3629$</td>
</tr>
<tr>
<td>Sphere 3D</td>
<td>$1 + \frac{\sqrt{8}}{3} \pi - \frac{5}{4} \pi \approx 3.49%$</td>
<td>$1.3519$</td>
</tr>
<tr>
<td>Random 2D</td>
<td>$\tilde{\theta} \in [49.12%, 60.84%]$</td>
<td>$b \in [0.8502, 1.4112]$</td>
</tr>
<tr>
<td>Random 3D</td>
<td>$\tilde{\theta} \in [29.56%, 35.56%]$</td>
<td>$b \in [0.8542, 1.0180]$</td>
</tr>
</tbody>
</table>

Also, the remaining models stated in (3.2) are reasonable approximations: The model $\theta^{4/3}$ by Millington & Quirk is appropriate for geometrical shapes lying somewhere in between the sphere and the cube. In 2D good agreement of upscaling results for the square, the cross type 2 and the relation given by Marshall for low porosities is obtained, cf. Figure 3.3. For high porosities Buckingham’s $\theta^2$ yields good values in the two-dimensional case for all considered geometries.

Moreover, the relation obtained from upscaling theory also fits very well for further, potentially anisotropic, specific situations. As already discussed in the context of *layered media* (being nothing but a system of straight *tubes*; cf. Section 3.3.2) a linear porosity–diffusion relation is obtained as well. Such a linear relation is represented in Figure 3.6 in the graph for rectangles leading to tube-like structures while growing. The investigations depicted in Figure 3.6 further demonstrate that the behavior of the two eigenvalues may be significantly different for anisotropic media. While one of the two eigenvalues shows, for instance, a linear dependency on porosity, the second eigenvalue evidently shows a monotonic but non-linear behavior. With these observations it is evident that the representation of the full *anisotropic diffusion tensor* by a scalar is not reasonable. The advantage of the put forward approach is that it also directly enables investigating anisotropic situations based on specific geometrical information.
Figure 3.8: Unconsolidated random distribution (left) and related consolidated
distribution (right) of solid (white) and pore space (blue) at a porosity
of 45%. Note that although the porosity is equal, the total surfaces
and the upscaled diffusion tensors are different.

The obtained numerical results from (3.4) for various, potentially anisotropic,
geometries are depicted in the Figures 3.3 – 3.7 and the related quantitative
functional dependences of $\frac{D_p}{D_0}$ are summarized in Table 3.1. For the random ge-
ometries, we investigate the eigenvalues for 100 unconsolidated and consolidated
samples for a porosity value of 0.45, cf. Figure 3.8. It is evident from Figure 3.9
that the resulting eigenvalues are always clustered and no arbitrary or uniform
distribution is obtained. More precisely, although we have some randomness in
the model, the effective response of the medium remains similar for a prescribed
porosity. This is also evident, since the approximating functions contain quite
small ranges for the parameters of 100 executions in Table 3.1. It is further of
note that the connectivity is much better in the three dimensional situation and
consequently the degeneration of the tensors is less prominent; compare the
values of $\hat{\theta}$ in Table 3.1 and also the evaluation of random geometries depicted
in Figure 3.7.

### 3.5.2 Evaluation of effective tensors over surface area

For the chosen representative geometries, the diffusion–total surface relation is
investigated in the following. The total surface area is — like in Section 2.2.4
— defined as surface scaled by the characteristic length (in two dimensions) or
characteristic area (in three dimensions) of an interface within the representative
Chapter 3  Predicting the diffusion in porous media

Figure 3.9: Frequency of eigenvalues for 100 executions of random scenarios with porosity of 45% in 3D. Here, the red, blue, and violet graphs depict the small, middle, and large eigenvalues of the homogenized diffusion tensors for random distributions, respectively. The green, brown, and gray graphs depict the respective eigenvalues, after the porosity preserving CAM as described in [3] has been executed.

Figure 3.10: Porosity $\theta$ over total surface $\sigma$ for isotropic geometries.

elementary volume. More precisely, we had definitions for:

- the total volume defined as the sum of the volumes of all solid particles, which is kept constant during our simulations.
- the total surface defined as the amount of cell interfaces which have a solid cell on one and a non-solid cell on the other side (scaled by the area of such an interface).

The relation between porosity $\theta$ and total surface $\sigma$ is shown in Figure 3.10. The advantage of the diffusion–total surface relation is that total surface may easily be related to pore size or grain size for simple geometries such as spheres. The latter ones are considered the primary controls rather than porosity alone for
3.5 Evaluation

Figure 3.11: Scalar $\frac{D_p}{D_0}$ over total surface $\sigma$ for isotropic geometries.

<table>
<thead>
<tr>
<th></th>
<th>$\sigma$ or eigenvalues of $\mathbb{D}/D_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Square 2D</td>
<td>$\tilde{\sigma} = 4$  $b \approx 1.2468$</td>
</tr>
<tr>
<td>Cross (type 1)</td>
<td>$\tilde{\sigma} = 4$  $b \approx 1.7399$</td>
</tr>
<tr>
<td>Cross (type 2)</td>
<td>$\tilde{\sigma} = 4$  $b \approx 1.3165$</td>
</tr>
<tr>
<td>Cube 3D</td>
<td>$\tilde{\sigma} = 6$  $b \approx 1.1654$</td>
</tr>
<tr>
<td>Random 2D (small EV)</td>
<td>$\tilde{\sigma} \in [30.7390, 34.6011]$  $b \in [1.2068, 1.5433]$</td>
</tr>
<tr>
<td>Random 2D (big EV)</td>
<td>$\tilde{\sigma} \in [31.6263, 35.3862]$  $b \in [1.2642, 1.6275]$</td>
</tr>
<tr>
<td>Random 2D agglo. (small EV)</td>
<td>$\tilde{\sigma} \in [17.3716, 19.8709]$  $b \in [1.5167, 2.1263]$</td>
</tr>
</tbody>
</table>

Table 3.2: Quantitative relations of $\frac{D_p}{D_0}$ or eigenvalues (EV) of $\mathbb{D}/D_0$ on the total surface $\sigma$. Note that the ansatz functions are $1 - \left(\frac{\sigma}{\tilde{\sigma}} \right)^b$.

general porous media. Similarly to the diffusion–porosity relations as investigated in Section 3.5.1, the diffusion–total surface relation is evaluated graphically in Figure 3.11 and functional relations are obtained via the approximation method described in Section 3.4, see Table 3.2.

Since the applied discretization method uses structured grids based on squares or cubes, all geometries are approximated by a composition of such cuboids. Therefore, especially the circle and the sphere but also other shapes (e.g. ellipse, octagon, hexagon) are not exactly represented within the chosen discretization. In the previous Section 3.5.1 this inaccuracy was marginal since the volume and hence the porosity of the exact shape and the approximating composition almost coincide. Contrarily, the total surface differs significantly. For instance, the exact circle with radius $\frac{1}{2}$ and related surface area of $\sigma = \pi$ touches the boundary of
the representative elementary volume. However, the approximation of such a circle by a composition of cuboids leads to a surface area of $4\pi$. Similarly in three dimensions, the surface area of the sphere is enlarged. Again the exact sphere touches the boundary of the unit cell if $\sigma = \pi$. This is in contrast to Figure 3.11 (right) where the maximal surface area of the sphere exceeds $4\pi$. Although less prominent, similar inaccuracies occur also for further geometries.

Nevertheless, the results provide a reasonable qualitative description. For instance, Figure 3.11 (left) shows a monotonically decreasing behavior for various geometries. From the figure it is evident that for a fixed surface area the lower the volume of a geometrical shape is (and hence the higher the porosity) the

Figure 3.12: Eigenvalues over total surface $\sigma$; each 100 executions of random scenarios for porosities in intervals of 5% in 2D (left) and 3D (right). Here, the red, blue, and violet graphs depict the small, middle and large eigenvalues of the homogenized diffusion tensors for random distributions, respectively. The green, brown, and gray graphs depict the respective eigenvalues, after the porosity preserving CAM as described in [3] has been executed. Black graphs are examples for suitable approximations.
bigger is the diffusion coefficient. Moreover, Figure 3.11 shows that contrarily to all other depicted geometries the diffusion coefficient does not degenerate when the surface area related to the spherical geometry becomes maximal in three dimensions, i.e. the sphere touches the boundary and starts overlapping. On the contrary, the diffusivity for the spherical geometry degenerates only for a radius of \( \frac{1}{\sqrt{2}} \) and surface area of \( \tilde{\sigma} = \left( \frac{6}{\sqrt{2}} - 4 \right) \pi \approx 0.762 \). Likewise, it is remarkable to note that also the diffusion–total surface relation of the three-dimensional unconsolidated random geometries does not degenerate when the surface gets maximal, cf. Figure 3.12 (right). The eigenvalues for 100 unconsolidated samples for a porosity value of 45\% (cf. Figure 3.8) are investigated in Figure 3.13. It is evident that the total surfaces for the realization lie in a small range and the corresponding eigenvalues do likewise. More precisely, although we have some randomness in the model, the effective response of the medium remains similar, cf. Figure 3.13.

The presented approach to quantitatively approximate the diffusion–total surface relation is already described in Section 3.4. Due to the significant inaccuracy of the surface area of the approximating composition of cuboids for some geometries only reasonable functional relations for well represented geometrical shapes are listed in Table 3.2.

Since the diffusion–surface relation is not monotinous for three-dimensional unconsolidated random geometries, the approach \( 1 - \left( \frac{a}{\tilde{\sigma}} \right)^b \) (ensuring that the slope in the origin is zero, i.e. \( \frac{\partial D_p}{\partial \tilde{\sigma}} (0) = 0 \)) is not useful in this particular case. Instead the eigenvalues of the diffusion tensor are approximated via \( \left( 1 - \frac{a}{\tilde{\sigma}} \right)^b \) (\( \tilde{\sigma} = 48, b = \frac{100}{378} \)) leading to \( \frac{\partial D_p}{\partial \tilde{\sigma}} (\tilde{\sigma}) = -\infty \), cf. Figure 3.12 (right).
3.5.3 Remark on tortuosity

Quintard concludes in [80] that porosity is the essential parameter only for unconsolidated, isotropic systems. However, detailed structural arrangement and composition play a crucial role in general porous media. Deriving various models, the assumption that a porous medium consists of straight tubes is made. Since it is evident that within a porous medium paths are in general no straight lines, the tortuosity is often integrated into the models to relax this assumption and overcome the related drawbacks. The prefactor 0.66 in the relation given by Penman in [79] is for instance interpreted in the following way: in realistic situations no straight tubes are present, such that the tortuosity must be accounted for and a reduction to $2/3 \approx 0.66$ is to be expected.

The tortuosity is defined as the ratio of the average traveling length per unit length. The following basic relations are often presupposed for the effective diffusion:

$$\frac{D_p}{D_0} = \frac{1}{\tau^2} \quad \text{and} \quad \frac{D_p}{D_0} = \frac{\theta}{\tau},$$

(3.8)

cf. [86, 95]. However, tortuosity is difficult to determine. Only for very sim-
ple situations, such as straight or perturbed channels, explicit relations may be obtained, cf. [84] in the context of diffusion. Ryan et al [83] considers 2D cubic inclusions and relates diffusion and tortuosity. Consequently, relations potentially also including the constrictivity $\delta$, resistivity factor $F$ or model parameters that may be calibrated with experimental data are available for tortuosity. Archie’s law $F = \frac{A}{\theta^m}$ (with parameters $A, m$) and further findings for instance suggest to relate the tortuosity to the porosity or some geometric shape factor, e.g. via

$$\tau^2 = (F\theta)^n = (A\theta^{(1-m)})^n$$

(3.9)

with parameters $A, m,$ and $n$, cf. [86]. A review of further expressions for the tortuosity $\tau = \tau(\theta)$ in terms of the porosity is given in [86], e.g.

$$\tau = \theta + B(1 - \theta) \quad \text{or} \quad \tau^2 = 1 - C \ln(\theta)$$

with parameters $B, C$. Possible choices for the parameters are discussed in [86]. The following examples demonstrate that a generally valid relation between porosity and tortuosity may not be expected. Considering the geometry on the left in Figure 3.14, with respect to the number of hills $\ell$, the porosity is given by $\theta = 1/32 + \ell \cdot 58/1024$ and the tortuosity lies in between the shortest and the longest traveling length, i.e. $\tau \in [1 + 1, 8135\ell, 1 + 1, 875\ell]$. In summary, the linear relation $\tau \approx -0,000 + 32,0176\theta$ between tortuosity and porosity is obtained. For the second geometrical setting as depicted in Figure 3.14 porosity remains constant, while tortuosity increases. Contrary to this, the geometrical setting sketched in the third picture in Figure 3.14 yields that the porosity increases while tortuosity decreases. The three examples show that the relation between tortuosity and the porosity may show significantly different behavior. For this reason, it is clear that many models, potentially comprising several parameters, have been proposed in the literature to describe the tortuosity–porosity relation in specific situations.

### 3.6 Conclusions and future prospects

In this chapter, well-established functional relations between porosity and effective diffusion are reviewed. Moreover, standard results from upscaling theory and related mathematical bounds are stated. For isotropic unconsolidated geometries, all approaches yield quite good results comparing the scalar diffusion. However, the approximation quality for anisotropic situations becomes worse. Moreover, fitting experimental data is restricted to small parameter ranges. The upscaling theory, however, enables calculating the full anisotropic tensor and allows covering larger parameter ranges. Additionally, quantitative relations between both diffusion and porosity, and diffusion and total surface are provided,
and the tortuosity–porosity relation is briefly surveyed. Another advantage of
the given approach is that no fitting parameters are needed. Only assumptions
on the underlying representative geometries are placed and fitting of functions
of type \( \left( \frac{\theta - \hat{\theta}}{1 - \hat{\theta}} \right)^b \) or \( 1 - \left( \frac{\sigma}{\hat{\sigma}} \right)^b \), respectively is undertaken. For approximations of the
diffusion–porosity relation by a function of type \( \varphi \theta^\xi \) as in (3.3), the exponent \( \xi \)
tries to compensate the neglected parameter \( \hat{\theta} \). Hence, it is rather big, cf. [90,
Table II], and the quality of approximation is worsened. Moreover, the full,
potentially anisotropic tensor (represented by its eigenvalues) is provided in the
presented approach instead of a scalar representative which is only reasonable
for isotropic situations.

Further studies may focus on quantitative relations for the diffusion tensor
similarly to Table 3.1 and Table 3.2, but for anisotropic settings. Moreover, it
would be of interest to obtain such relations on total surface and diffusion for
curved geometries (e.g. circle, sphere) either by a rescaling argument or by
avoiding the discretization inaccuracy described in Section 3.5.2. Also, fitting
the data to polynomials \( \sum_k a_k x^k \) or other functional relations may certainly be
worth investigating. Further research may also investigate relations based on
additional geometric characteristics such as the mean grain size. Finally, the
comparison to experimental data is an important aspect for future research.

Although diffusion is certainly of great interest in many applications, dispersion
and the related diffusion–dispersion coefficient are relevant for dominant flow
regimes. This is topic of further research. Based on current findings, similar
considerations as in the present chapter will be done for the permeability–porosity
relation and discussed in the context of Kozeny–Carman. Finally, additional re-
search including extensions of homogenization results is needed to similarly
approach flow and diffusive transport in the unsaturated case.

Another important aspect to take into account for a comprehensive model is
the specific cause leading to a dynamic change of porosity. Such a model for
porosity change can then be used in conjunction with the current model for the
diffusion–porosity relation. One area of application resulting in the dynamic
change in porosity are precipitation–dissolution reactions at the solid–liquid
interface \( \partial Y_s \).

Along the line of upscaling diffusion for evolving microstructures, we still
have to investigate the influence of the discretely moving solid domain in the
model of Chapter 2. This is done in the following chapter.
Chapter 4

Analysis of homogenization for discontinuous tensors

Abstract of the chapter. The aim of this chapter is to provide a justification for the modeling assumption in Chapter 2 that the movement of e.g. solid particles on the micro-scale only happens at discrete points of time. For this purpose, we assume the movement on the micro-scale to take place at distinct — but comparably short — time-intervals, while the modeled effects on the macro-scale are assumed to be continuous with respect to time.

Outline of the chapter. We proceed as follows: In Section 4.1, the problem is illustrated, and a mathematical formulation of the problem is presented. Section 4.2 is devoted to the analysis of the problem with an at most countable number of jumps before formal temporal homogenization is conducted in Section 4.3. Short conclusions and future prospects wrap up this chapter.

4.1 Motivation and formulation of the problem

Illustrating the behavior of the model in Chapter 2, we restrict ourselves to the case of only one time-interval, when movement on the micro-scale takes place. Additionally, we consider the model where we only have solid particles and a fluid phase (i.e., no gas phase, no biomass, ...). Nevertheless, all arguments produced in the following can easily be transferred to the case of the full model. Thus, from the initial time $t_0 \geq 0$ to $t_- > t_0$ no particles are allowed to move, at $t_-$ (the starting time for the movement on the micro-scale) all particles move, and after $t_+ > t_-$ (the final time of movement on the micro-scale) they are not allowed to move again. In other words, we have three temporal sub-intervals describing the problem $(P_\tau)$:
1. In \([t_0, t_-] \) no particles are allowed to move. This can be interpreted as the solid matrix being fixed, while time proceeds. The spatial configuration of solid particles in this time-interval is denoted by \(\text{Config}^{(1)}\).

2. In \([t_-, t_+] \) with \(t_+ := t_- + \tau\) the particles move. This can be interpreted as the time interval of length \(\tau\), when the solid matrix is allowed to restructure. From a physical point of view, the movement of particles is supposed to be continuous, but for mathematical analysis this is not necessary.

3. In \((t_+, T] \) no particles are allowed to move again. This can be interpreted as the solid matrix being fixed, while time proceeds. The spatial configuration of solid particles in this time-interval is denoted by \(\text{Config}^{(2)}\).

Here, \(t_0\) can be interpreted as initial time, while \(\tau\) is the length of the time period of movement and \(T\) is the final time of our experiment. In this context, our model approach can be interpreted as assuming that the microstructure (configuration of solid blocks) is constant in \([t_0, t_-)\) and \((t_+, T]\).

From a physical / soil scientific point of view, one might think of an earthworm digging through earth or other rather short events (earthquakes, high precipitation, freezing, quick drying) changing the soil’s matrix in a rather short period of time compared to the time of observation.

Only interested in the behavior of some macroscopic variable (e.g. concentrations of substances distributed in the porous medium) in a temporal sense, we will investigate whether it is necessary to model the changes in the soil matrix (in their temporal development), or whether it is enough to know the state of the soil matrix before and after the reconfiguration, i.e. \(\text{Config}^{(1)}\) and \(\text{Config}^{(2)}\). We hope (and will find out) that we can neglect modeling the temporal development of the soil matrix if we want to know the evolution of some macroscopic variable. This can be interpreted as some sort of homogenization with respect to time.

Thus, we introduce a set of problems \((P_\tau)_{\tau \in [0, \tau]}\) (with \((P_\tau) = (P_\tau)\) if \(\tau = \tau\)), satisfying the following properties for all \(\tau \in [0, \tau]\), and \(t_+ := t_- + \tau\):

1. In \([t_0, t_-) \) the spatial configuration of particles is \(\text{Config}^{(1)}\).

2. In \([t_-, t_+] \) with \(t_+ := t_- + \tau\) the particles move.

3. In \((t_+, T]\) the spatial configuration of particles is \(\text{Config}^{(2)}\).

Moreover, we have to assume that for all \(t \in [t_0, T], \tau \in [0, \tau]\) the configuration of solid particles induces a symmetric positive semi-definite, upscaled (with respect to the spatial variables) diffusion tensor which is necessary for our
4.2 Analysis of the problem with countable jumps

To analyze the given problem, we start with formulating the system in a more rigorous way: Let \( \Omega \subset \mathbb{R}^d \) be a bounded Lipschitz-domain and \( T > t_0 \). We will discuss the following initial and boundary value problem:

$$
\begin{cases}
\partial_t u_{\tau} - \nabla \cdot (D_\tau \nabla u_{\tau}) = f & \text{in } (t_0, T) \times \Omega, \\
u_{\tau}(t_0, x) = u_{\text{start}}(x) & \text{in } \Omega, \\
u_{\tau} = u_D & \text{on } (t_0, T) \times \Gamma_D, \\
-D_\tau \nabla u_{\tau} \cdot \nu = g_N & \text{on } (t_0, T) \times \Gamma_N
\end{cases}
$$

(4.1)

representing \((P_{\tau})\) for \( \tau > 0 \) should in some sense converge towards the solution \( u_0 \) of the problem

$$
\begin{cases}
\partial_t u_0 - \nabla \cdot (D_0 \nabla u_0) = f & \text{in } (t_0, T) \times \Omega, \\
u_0(t_0, x) = u_{\text{start}}(x) & \text{in } \Omega, \\
u_0 = u_D & \text{on } (t_0, T) \times \Gamma_D, \\
-D_0 \nabla u_0 \cdot \nu = g_N & \text{on } (t_0, T) \times \Gamma_N
\end{cases}
$$

(4.2)

which is the corresponding macroscopic equation for \( \tau = 0 \) and problem \((P_0)\) on the macroscopic domain \( \Omega \). The given data of (4.1) and (4.2) is identical, except for the diffusion tensor which is only allowed to be different in \([t_-, t_+].\)

Moreover — remembering the very first paragraph of this chapter — the above described convergence should still hold true if we allow for a countable amount of discrete jumps and the case that the first jump happens at \( t_- = t_0 \). In contrast to this, the case that the last jump happens at \( t_- = T \) is trivial.

However, it is important to note that the assumption about time scales (discrete movement being fast compared to continuum transport) is only justified in regimes when the microaggregates are quasi static, i.e., it cannot be applied directly to the modeling of microaggregate formation.
Chapter 4 Analysis of homogenization for discontinuous tensors

Problem 4.2.1. Let \( \partial \Omega = \Gamma_D \cup \Gamma_N \) (disjoint union). We seek a family of functions \( u_\tau \in H^1(t_0, T; H^*(\Omega)) \cap L^2(t_0, T; H^1_{\Gamma_D}(\Omega, u_D)) \) such that

\[
\begin{aligned}
\partial_t u_\tau - \nabla \cdot (D_\tau \nabla u_\tau) &= f & \text{in } (t_0, T) \times \Omega \\
\quad & \text{in } \Omega \\
\quad & u_\tau(t_0, x) = u_{\text{start}}(x) & \text{on } (t_0, T) \times \Gamma_D \\
\quad & u_\tau = u_D & \text{on } (t_0, T) \times \Gamma_N \\
-D_\tau \nabla u_\tau \cdot \nu &= g_N & \text{on } (t_0, T) \times \Gamma_N
\end{aligned}
\]  

(4.3)

for given \( f \in L^2(t_0, T; H^*(\Omega)) \), \( D_\tau \in L^\infty(t_0, T; L^\infty(\Omega)^{d,d}) \) uniformly symmetric positive semi-definite, \( u_D \in H^1(t_0, T; H^{1/2}(\partial \Omega)) \), \( g_N \in L^2(t_0, T; (H^{1/2}(\partial \Omega))^\tau) \), \( \tau \in [0, \overline{T}], \overline{T} > 0 \). \( u_{\text{start}} \) has to be as regular as \( u_D \) with respect to space and the boundary conditions have to hold for \( u_{\text{start}} \).

Remark 4.2.2 (Notation and function spaces). For the (non-empty, open) domain \( \Omega \), the spaces \( L^p(\Omega) \) with \( 1 \leq p \leq \infty \) denote the standard Lebesgue spaces on \( \Omega \) and \( H^k(\Omega) \) for \( k \in \mathbb{N} \) denotes the standard Sobolev spaces. In the rest of this thesis, the trace space \( H^{1/2}(\partial \Omega) \) shall further be defined as the image of the trace operator \( \gamma_0 \), as presented in [104, p. 130]. Moreover, \( H^m_{\Gamma_D}(\Omega, u_D) := \{ u \in H^m(\Omega) : \gamma_0|_{\Gamma_D}(u) = u_D \}, C^\infty_{\Gamma_D}(\overline{\Omega}, 0) := C^\infty(\overline{\Omega}) \cap H^1_{\Gamma_D}(\Omega, 0) \), and \( H^*(\Omega) := \left( H^1_{\Gamma_D}(\Omega, 0) \right)' \). A similar space is defined in [100, Sect. 5.9.1]. Beyond this, for \( a, b \in \mathbb{R}, a < b \) and a Banach space \( X \), the spaces \( L^2(a, b; X) \), \( H^k(a, b; X) \) are the standard Bochner spaces [100, Sect. 5.9.2]. For further details about these space, the reader may consult [100, 103].

Remark 4.2.3.

1. Obviously, there is a constant \( C_D > 0 \) (independent of \( t \in [t_0, T] \), \( x \in \Omega \), and \( \tau \)) such that for all \( \xi \in \mathbb{R}^d \)

\[
\xi \cdot D_\tau \xi \leq C_D \|\xi\|_2^2.
\]

2. Additionally, we assume that all \( u_\tau \) are uniformly bounded in the sense that there is a \( \overline{C} > 0 \) and a \( \delta > 0 \) such that \( \|u_\tau\|_{L^{2+\delta}(t_0, T; H^1(\Omega))} \leq \overline{C} \) for all \( \tau \geq 0 \). This can for example be deduced under the additional preconditions in [100, Theorem 5.1, p. 360] for smooth \( \Omega \) with a slightly adapted proof exploiting the uniform properties of \( D_\tau \). However, this assumption is not always met even in large scale simulations.

We need a weak version of our problems. Hence, we define smooth test functions \( \varphi \in H^1(t_0, T; C^\infty_{\Gamma_D}(\overline{\Omega}, 0)) \), multiply (4.3) by these test functions and integrate by parts. Thus we get for almost every \( s \in [t_0, T] \)

\[
\int_\Omega \partial_t u_\tau \varphi \, dx + \int_\Omega D_\tau \nabla u_\tau \cdot \nabla \varphi \, dx + \int_{\Gamma_N} g_N \varphi \, d\sigma = \int_\Omega f \varphi \, dx.
\]  

(4.4)
This equation will be the basis of our analysis. Therefore, it might be interesting to read about the existence and regularity of (unique) solutions of these equations. This can be done in [100–103]. For us, it is enough to realize that there is a unique solution. In the following, we want to show that we have convergence for \( \tau \downarrow 0 \) and a countable amount of jumps. To do so, we consider a countable set of jumps at discrete points of time \((t_i)\), having total length \(\tau\).

**Theorem 4.2.4.** The solutions \( u_\tau \) converge to \( u_0 \) for \( \tau \downarrow 0 \) in the sense that for almost every \( s \in [t_0, T] \)

\[
\|u_\tau(s, \cdot) - u_0(s, \cdot)\|^2_{L^2(\Omega)} + \int_{t_0}^s \|\sqrt{D_\tau} (\nabla u_\tau - \nabla u_0)\|^2_{L^2(\Omega)} \, dt \downarrow 0 \quad \text{for} \quad \tau \downarrow 0.
\]

**Proof.** Since \( C_\infty^0(\Omega, 0) \) is dense in \( H^1_\Gamma D(\Omega, 0) \) with respect to \( \| \cdot \|_{H^1(\Omega)} \), we can choose \( \varphi = u_\tau - u_0 \). Now we define \( \overline{u} = u_\tau - u_0 \), subtract the equations (4.4) (for \( \tau > 0 \) and \( \tau = 0 \) from one another), and perform simple algebraic manipulations to gain:

\[
\int_{t_0}^s \frac{1}{2} \int_\Omega \partial_t \left( \overline{u}^2 \right) \, dx \, dt + \int_{t_0}^s \int_\Omega D_\tau \nabla \overline{u} \cdot \nabla \overline{u} \, dx \, dt \\
= \int_{t_0}^s \int_\Omega (D_0 - D_\tau) \nabla u_0 \cdot \nabla \overline{u} \, dx \, dt \\
\leq \int_{t_0}^s \|D_0 - D_\tau\|_{L^\infty(\Omega)} \|\nabla u_0\|_{L^2(\Omega)} \|\nabla \overline{u}\|_{L^2(\Omega)} \, dt \\
\leq 2C_D \int_{t_0}^s \|\nabla u_0\|_{L^2(\Omega)} \|\nabla \overline{u}\|_{L^2(\Omega)} \, dt \\
\leq 2C_D \|u_0\|_{L^{2+\delta}(t_0, T; H^1(\Omega))} \|\overline{u}\|_{L^{2+\delta}(t_0, T; H^1(\Omega))} \|u_0\|_{L^{2+\delta}(t_0, T; H^1(\Omega))} \|\nabla \overline{u}\|_{L^2(\Omega)} \, dt \\
\leq 4C_D \overline{C}_D^2 \tau^{\frac{\delta}{2}} \tau^{\frac{\delta}{2}},
\]

where we heavily relied on *Hölder’s inequality*. This gives the result. \( \square \)

### 4.3 Temporal homogenization by asymptotic expansion

Having analyzed the case of a countable amount of jumps, we now turn to the case that \( D \) has periodic oscillations at every single point of time (which we only treat formally). More precisely, we consider the case that \( D^\epsilon \) has periodic oscillations of length \( \epsilon \) and try to construct a temporally homogenized setting by
considering \(\varepsilon \searrow 0\). Proceeding as in standard upscaling theory, we formulate the problem

\[
\begin{align*}
\partial_t u^\varepsilon - \nabla \cdot (D^\varepsilon \nabla u^\varepsilon) &= f & \text{in } (t_0, T) \times \Omega, \\
u^\varepsilon(t_0, x) &= u_{\text{start}}(x) & \text{in } \Omega, \\
u^\varepsilon &= u_D & \text{on } (t_0, T) \times \Gamma_D, \\
-\nabla u^\varepsilon \cdot \nu &= g_N & \text{on } (t_0, T) \times \Gamma_N.
\end{align*}
\]

Asymptotic expansion yields for the scalar \(\tau := \frac{t}{\varepsilon}\)

\[
u^\varepsilon(t, x) = u^0(t, \frac{t}{\varepsilon}, x) + \varepsilon u^1(t, \frac{t}{\varepsilon}, x) + \ldots,
\]

\[D^\varepsilon(t, x) = D^0(t, \frac{t}{\varepsilon}, x) + \varepsilon D^1(t, \frac{t}{\varepsilon}, x) + \ldots.\]

The functions \(u^k, k \in \mathbb{N}\) depend on the two temporal variables \(t\) ("macroscopic" large time) and \(\tau \in Y := [0, 1]\) ("microscopic" short time). (Note that similar notation with different meanings for functions with one and two temporal variables is used!) Thus, \(\partial_t\) transforms to \(\partial_t = \partial_t + \frac{1}{\varepsilon} \partial_{\tau}\) and the lowest order problem is time-independent, since

\[
\partial_{\tau} u^0 = 0 \quad \text{in } (t_0, T) \times Y \times \Omega, \quad \text{i.e.} \quad u^0(t, \tau, x) = u^0(t, x).
\]

Hence, the zeroth order problem can be formulated as

\[
\begin{align*}
\partial_t u^0 - \nabla \cdot (D^0 \nabla u^0) &= f - \partial_{\tau} u^1 & \text{in } (t_0, T) \times Y \times \Omega, \\
u^0(t, \tau, x) &= u_{\text{start}}(\tau, x) & \text{in } Y \times \Omega, \\
u^0 &= u_D & \text{on } (t_0, T) \times Y \times \Gamma_D, \\
-\nabla u^0 \cdot \nu &= g_N & \text{on } (t_0, T) \times Y \times \Gamma_N
\end{align*}
\]

and integration over \(Y\) with respect to \(\tau\) yields

\[
\partial_t u^0 - \nabla \cdot (D^0 u^0) = f - \int_Y \partial_{\tau} u^1 \, d\tau = f - (u^1(t, 1, x) - u^1(t, 0, x)) = f,
\]

since \(u^1\) is \(Y\)-periodic. Here, \(D(t, x) = \int_0^1 D^0(t, \tau, x) \, d\tau\) represents the macroscopic diffusion tensor of the temporally homogenized problem.

### 4.4 Conclusions and future prospects

In this chapter, we briefly underlined that there are no problems to be expected from the fact that the model in Chapter 2 combines both, temporally discrete jumps and spatial homogenization. Nevertheless, a more rigorous investigation of temporal homogenization using two-scale convergence would be interesting. Additionally, the question arises whether and under which conditions the limits appearing in temporal and spatial homogenization can be interchanged.
Chapter 5

Analysis of the discontinuous Galerkin method for Darcy’s equation

Abstract of the chapter. This chapter aims at showing that the local discontinuous Galerkin method is a good choice of discretization scheme for the model of Chapter 2 describing the development of microaggregates. Moreover, extensions of the method are analyzed that are capable of increasing performance and/or improving accuracy.

In addition, it presents a new version of the local discontinuous Galerkin method capable of dealing with jump conditions along a submanifold $\Gamma_{LG}$ (i.e. Henry’s law) in instationary Darcy flow. The analysis accounts for a spatially and temporally varying, non-linear permeability tensor in all estimates — allowed to have a jump at $\Gamma_{LG}$ — and gives a convergence order result for the primary and the flux unknowns. In addition to this, different approximation spaces for the primary and the flux unknowns are investigated. The results imply that the most efficient choice is to select the degree of the approximation space for the flux unknowns one less than that of the primary unknown. The only stabilization in the proposed scheme is represented by a penalty term in the primary unknown.

Additionally, this scheme is applied to and analyzed for the non-linear advection–diffusion equation, and a hybridizable discontinuous Galerkin method for parabolic equations with non-linear tensor-valued coefficients and jump conditions is formulated. The analysis of the latter indicates the optimal convergence order that is confirmed to be sharp in numerical studies. A series of numerical experiments investigates the effect of choosing different order approximation spaces for different unknowns.

The notation of this chapter relies on the notation introduced in Remark 4.2.2.

Outline of the chapter. The following text is structured as follows: First, in Section 5.1, an overview of existing discontinuous Galerkin schemes, their re-
Section 5.2 presents a local discontinuous Galerkin scheme capable of dealing with jumps — both in the unknown and in the coefficient in the transport equation appearing at phase transitions of the model in Chapter 2. The flexibility of this scheme is demonstrated in Section 5.3 by applying it to an advection–diffusion equation. In Section 5.4, the scheme is hybridized, and the resulting hybrid local discontinuous Galerkin method is analyzed before Section 5.5 wraps up the chapter by summarizing its results.

Previously published articles. Large parts of Section 5.2 have already been published in


and use results and expressions from


Section 5.3 has been created by Andreas Rupp, Vadym Aizinger, Balthasar Reuter, and Peter Knabner. Most parts of Section 5.4 have been submitted to a scientific journal and are expected to be published in a joint article by Markus Musch, Andreas Rupp, Vadym Aizinger, and Peter Knabner.

### 5.1 Introduction and motivation

The *discontinuous Galerkin (DG)* method first introduced in [158] for a transport equation has become one of the most widely used numerical schemes in many areas of computational fluid dynamics (CFD). Particularly important for a wide adoption of this method was the appearance of discretization techniques for second order terms such as the Laplace operator. Those techniques currently include:
• discretizations operating directly on the scalar partial differential equation (PDE) similarly to the classical finite element method that originate from the interior penalty (IP) schemes introduced in the late 1970s and early 1980s for elliptic and parabolic equations (cf. [109] for an overview);
• DG methods based on the mixed formulation, in particular the local discontinuous Galerkin (LDG) method first introduced by Cockburn and Shu for convection–diffusion systems in [124];
• DG discretizations using staggered approach for flux reconstruction [141].

The mixed DG formulations — also considered in the present work — replace each second (or higher) order equation with a first order system by introducing auxiliary flux variables. In addition, this type of DG discretization is the foundation of the compact discontinuous Galerkin (CDG) [155] and the hybridized discontinuous Galerkin (HDG) [115] methods. For an overview of the current state of development of DG methods and of DG formulations for various types of applications, the interested reader may consult a number of excellent review articles [121, 153, 162, 163, 169, 171].

The original work by Cockburn and Shu [124] on the LDG method for the convection–diffusion equation with constant coefficients considers a symmetrized mixed formulation distinctly differing from the approach of this thesis. A corresponding elliptic problem is analyzed in great detail in [117] where some sharp convergence results for the primary and the flux unknowns are presented for the first time. The analysis in [117] considers the Poisson equation, and the estimates for the primary and the flux unknowns are conducted separately producing convergence rates of $O(h^{k+1})$ and $O(h^k)$ in the $L^2$-norm, respectively for equal-order approximations of order $k$ for both unknowns. A Fourier-type analysis (performed by re-casting one-dimensional DG discretizations as finite differences stencils) is demonstrated by Zhang and Shu in [170]. Dawson in [131] presents an LDG scheme (whose formulation also includes some reconstruction ideas) based on approximation spaces one order higher for the flux variables proving convergence rates of $O(h^{k+1})$ for all unknowns. Similar LDG methods are also investigated in [107, 118].

Analysis of numerical methods for Darcy flow usually considers a somewhat more general setting than a classical (linear) diffusion equation or Poisson problem. The important issues for this specific application include spatially and (possibly also temporally) varying tensor-valued coefficients; the studies also should ideally evaluate the behavior of the numerical method in cases of discontinuous permeability. An intermediate step between a constant diffusion and the full Darcy problem in the case of the LDG method was covered by the work of Cockburn and Dawson [123] where a space/time variable non-negative diffusion coefficient was analyzed for the first time. Methods for Darcy flow have
been formulated and analyzed in the well-known paper by Brezzi et al. [111] that also discusses the well-posedness of the proposed DG formulation; the scheme presented there is stabilized by a residual-based approach based on ideas in [147] and [140] and works for polynomial orders \( k \geq 1 \). Other discontinuous Galerkin methods for Darcy flow are examined in [166], a more general problem is analyzed in [165]. Similar ideas as in [111] augmented by \textit{a posteriori} error estimates are investigated in [110].

Somewhat closer to the present study is the work of Perugia and Schötzau [156] where an \( hp \)-error analysis of an LDG method for \textit{stationary diffusion problems} with variable coefficients is carried out. Their analysis relies on test functions similar to ours; however the non-symmetric formulation of the second-order term is dealt with by introducing a third auxiliary unknown (reminiscent of [107]) instead of the direct approach used here, also the stabilization terms of order \( O(h^{-1}) \) similar to [117] are employed.

Most of the above mentioned DG methods have been around for several decades. They have a number of well-known advantages compared to the classical \textit{finite element methods (FEM)} such as natural support for \textit{non-conforming meshes} and \textit{hanging nodes}, \textit{hp}-\textit{adaptivity}, \textit{local mass conservation}, etc. Their major drawback is a significantly greater number of \textit{degrees of freedom} than in finite element discretizations of the same order. A recent development, the \textit{hybridized discontinuous Galerkin (HDG)} methods first proposed by Cockburn and co-workers in 2008 – 2009 [127, 130] aim to remedy this disadvantage while retaining the advantages of traditional DG methods. Furthermore, HDG methods possess other highly desirable properties such as optimal convergence and even super-convergence (of some parts of solutions such as local mean values or local fluxes), which can be exploited by post-processing techniques (see [150] for an overview of the early developments of the HDG methods).

The aforementioned advantages of the HDG methodology gave rise to a large number of applications to different problems. To name just a few: \textit{incompressible Stokes} [151] and \textit{Navier–Stokes} [152] equations, \textit{Maxwell equations} [154], \textit{linear elasticity} [133], \textit{linearized shallow-water equations} [112]. Furthermore, comparisons of \textit{accuracy}, \textit{robustness}, and \textit{computational efficiency} between HDG and DG [143, 168], HDG and classical FEM [144], HDG and \textit{finite volumes} [106] also received some attention.

Moreover, the class of \textit{hybrid high-order methods} based on hybridizing the primal formulation leads to a rather simple error analysis on polytopic meshes where only \( L^2 \) projections are used (as opposed to the rather complicated projection in the following). This is achieved by a novel stabilization design (cf. [133]). For recent developments in hybrid high-order and HDG methods, the reader may consult [113, 157].
Here, the main interest in connection with HDG schemes concerns the flow and transport in porous media, where DG methods have shown to be very useful. Their affinity to unstructured meshes and adaptivity are useful properties for complex geometries encountered in real-world problems [3]. Another feature distinguishing the HDG schemes from their DG counterparts is the convergence for approximation spaces of order zero. This capability is often desirable in the context of porous media, where many simulators utilize lowest order spaces (cf. [161]). However, in a decade of development, only a few studies focusing on porous media problems appeared in the HDG literature [138, 161].

The DG schemes presented in this work are stabilized using penalties in the primary unknown, and thus fit into the unified DG framework established in [109]. The strengths of the demonstrated approach include using the “traditional” type of DG analysis and a “natural” DG norm to simultaneously obtain convergence results for both, the primary and the flux unknowns. All estimates incorporate variable, non-linear diffusion/permeability coefficients and inhomogeneous Dirichlet and Neumann boundary conditions.

5.2 A local discontinuous Galerkin scheme for Darcy’s equation including jump conditions and using different approximation spaces

Jump conditions at interfaces are widely used to model the coupling of flow and transport between subsurface and overland flows [164], incompressible two-phase flows with different densities [105], different compartments within cells and different cells themselves [142], different phases within concrete [149], or different phases within soil [108] with a transmission condition modeled by Henry’s law.

The local discontinuous Galerkin (LDG) method introduced by Cockburn and Shu in [124] uses a symmetrized, mixed formulation and tends to have problems with such systems since solutions with jump conditions are not in \((H^1, H^\text{div})\) and the analysis of the LDG method usually needs enough regularity such that traces on element boundaries are well-defined. In this thesis, the proposed method uses a non-symmetric approach to discretize the Darcy flux \(q = -D(u)\nabla u\). Dawson showed in [131] that using \(p^{k+1} - S^k\) discontinuous Galerkin methods could increase the order of convergence in both variables. A similar approach will also be investigated in the following, but here the higher order space is for the primary unknown, in contrast to the scheme presented in [131].

A different approach for a similar problem can be found in [137].
5.2.1 Problem formulation

We analyze an LDG method for an instationary Darcy problem on a bounded Lipschitz domain \( \Omega \subset \mathbb{R}^d \) which is assumed to be subdivided into two open, disjoint, non-degenerated, Lipschitz polytopes \( \Omega^l, \Omega^g \) such that \( \overline{\Omega} = \overline{\Omega^l} \cup \overline{\Omega^g} \). We assume \( \partial \Omega \) to be disjointly subdivided into \( \Gamma_D \) and \( \Gamma_N \) denoting the Dirichlet and Neumann boundaries, respectively. Moreover, \( \Gamma_{LG} := \partial \Omega^l \cap \partial \Omega^g \) is the boundary between \( \Omega^g \) and \( \Omega^l \) where the Henry jump condition is supposed to hold. A sketch of a simple \( \Omega \) satisfying all the above conditions is depicted in Figure 5.1. The problem can be formulated as follows:

\[
\begin{align*}
\partial_t u + \nabla \cdot q &= f \quad \text{in} \quad (0,T) \times (\Omega^l \cup \Omega^g), \\
D^{-1}(u)q + \nabla u &= 0 \quad \text{in} \quad (0,T) \times (\Omega^l \cup \Omega^g), \\
u^l / u^g &= H^l \quad \text{on} \quad (0,T) \times \Gamma_{LG}, \\
q^l \cdot v^l + q^g \cdot v^g &= 0 \quad \text{on} \quad (0,T) \times \Gamma_{LG}, \\
q \cdot v &= g_N \quad \text{on} \quad (0,T) \times \Gamma_N, \\
u &= u_D \quad \text{on} \quad (0,T) \times \Gamma_D, \\
u(0,x) &= u_0(x) \quad \text{in} \quad \Omega^l \cup \Omega^g, 
\end{align*}
\]

(5.1)

for given \( D^{-1}(\cdot) \in L^\infty(0,T;W^{1,\infty}(\Omega^l \cup \Omega^g)^d,d) \) strongly Lipschitz and uniformly symmetric positive definite with inverse \( D(\cdot) \in L^\infty(0,T;W^{1,\infty}(\Omega^l \cup \Omega^g)^d,d) \), \( H^l \in \mathbb{R}^+ \), \( f \in L^2(0,T;L^2(\Omega)) \), and \( u_D, g_N \in L^2(0,T;H^1(\Omega^l \cup \Omega^g)) \). Here and in the following, \( v^\alpha \) denotes the outward unit normal with respect to \( \Omega^\alpha \) (\( \alpha = l, g \)) and \( v \) is the outward unit normal with respect to \( \Omega \).

In this problem (interpreted in the context of Section 2.2.2), the dimensionless solubility constant \( H^{LG} \) describes the ratio between the aqueous concentration \( u^l \) and the gas concentration \( u^g \) of a chemical species.

Remark 5.2.1.

1. In this work, \( D(\cdot), D^{-1}(\cdot) \) being strongly Lipschitz means that there is a
5.2 A LDG scheme for Darcy’s equation including jump conditions

canonical $L_D > 0$ such that for all $v, w \in L^2(\Omega)$
$$
||D^{-1}(v) - D^{-1}(w)||_{L^2(\Omega)^d} \leq L_D ||v - w||_{L^2(\Omega)}
$$
and
$$
||D(v) - D(w)||_{L^2(\Omega)^d} \leq L_D ||v - w||_{L^2(\Omega)}.
$$
2. $D(\cdot), D^{-1}(\cdot)$ being uniformly symmetric positive definite is equivalent to the existence of a constant $C_D \geq 1$ (independent of $u \in L^2((0, T) \times \Omega)$, $t \in (0, T)$ and $x \in \Omega^1 \cup \Omega^g$) such that for all $\xi \in \mathbb{R}^d$
$$
C_D^{-1} ||\xi||_2^2 \leq \xi \cdot D(u)\xi \leq C_D ||\xi||_2^2,
$$
This implies $C_D \geq \|D(u)(t, \cdot)\|_{L^\infty(\Omega^1 \cup \Omega^g)}$ and $C_D \geq \|D^{-1}(u)(t, \cdot)\|_{L^\infty(\Omega^1 \cup \Omega^g)}$.
3. We can also allow for $\Phi, \partial u$ as the first term, where $\Phi \in L^\infty(0, T; W^{1, \infty}(\Omega))$ and $\Phi(t, x) \geq \Phi_0 > 0$ for a.e. $t \in (0, T)$ and a.e. $x \in \Omega$.
4. The flux unknown $q = -D(u)v$ can be interpreted as Darcy flux and its “continuity” across $\Gamma_{LG}$ ensures “conservation of mass”, while the primary unknown $u$ can be interpreted as hydraulic head.
5. One could also choose $u_D \in L^2(0, T; H^{1/2}(I_\Omega \cap \Omega^1) \cup (I_D \cap \Omega^g))$ and $g_N \in L^2(0, T; H^{1/2}(\Gamma_N))$, but should note that $u_D$ has to fulfill a consistency condition with respect to Henry’s law. That is, $u_D$ has to be a function which suffices Henry’s law or the trace of such a function.
6. In the above equations, $\Gamma_{LG}$ is supposed to be piecewise linear. If this does not hold true and the domains cannot be meshed exactly anymore, but $\Gamma_{LG}$ is smooth enough for traces to be well-defined, an additional error representing the mismatch between computational mesh and domain has to be considered. For alternative approaches considering unfitted interfaces, please I refer to [114].

Having defined our problem we now have to say what properties a weak solution of the above problem is assumed to have:

**Definition 5.2.2 (Weak solution and regularity).** A weak solution of (5.1) on the domain $\Omega$ is defined as $(u, q) \in \left(L^2((0, T) \times \Omega), L^2((0, T) \times \Omega)^d\right)$ that fulfills the following conditions:

1. For $\alpha = 1, g$ the restriction of $u$ on $\Omega^\alpha$ has the following properties:
   $$
u^\alpha \in H^1(0, T; L^2(\Omega^\alpha)), \quad u^\alpha \in L^2(0, T; H^1(\Omega^\alpha)).$$
   For the solution $u$ being in $H^1$ in both parts of the domain with traces that suffice the Henry condition, the function
   $$
   \tilde{u} = \left\{ \begin{array}{ll}
u^1 & \text{in } (0, T) \times \Omega^1 \\
H^{\Gamma_{LG}} u^g & \text{in } (0, T) \times \Omega^g
\end{array} \right.
   $$
   (5.2)
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is in $H^1(\Omega)$, since its traces are equal on $\Gamma_{LG}$.
2. The function $q^\alpha$ is an element of $L^2(0,T;H^1(\Omega^\alpha)^d)$ for $\alpha = 1, g$. This
implies (as a requirement) that $q$ is an element of $L^2\left(0,T;H^2_{\text{div}}(\Omega)\right)$.
3. The following equations have to be satisfied for any smooth test function $\varphi_u \in C^\infty((0,T) \times \Omega)$ or $\varphi_q \in C^\infty((0,T) \times \Omega)^d$, and for a.e. $t \in (0,T)$:

$$\int_{\Omega} \partial_t u \varphi_u \, dx - \int_{\Omega} q \cdot \nabla \varphi_u \, dx + \int_{\Gamma_D} g \varphi_u \, d\sigma - \int_{\Omega} f \varphi_u \, dx = 0,$$

$$\int_{\Omega} D^{-1}(u) q \cdot \varphi_q \, dx - \int_{\Omega} u \left(\nabla \cdot \varphi_q\right) \, dx + \int_{\Gamma_{LG}} (u^1 - u^g) \varphi_q \cdot \nu^1$$

$$+ \int_{\Gamma_N} u \varphi_q \cdot \nu \, d\sigma + \int_{\Gamma_D} u \varphi_q \cdot \nu \, d\sigma = 0,$$

$$\int_{\Omega} u(0,x)\varphi_u(0,x) \, dx - \int_{\Omega} u_0(x)\varphi_u(0,x) \, dx = 0.$$

The weak solution $(u, q)$ is said to be $(\bar{k}, k)$-regular, if $u^\alpha \in L^2\left(0,T;H^\bar{k}(\Omega^\alpha)\right)$ and $q^\alpha \in L^2\left(0,T;H^k(\Omega^\alpha)^d\right)$ for $\alpha = 1, g$, and $k$-regular if $k = \bar{k}$.

The equations in Definition 5.2.2 are constructed by multiplying (5.1) with smooth test functions, integration, and integration by parts. One could also define equivalent equations using $\hat{u}$: In this case the integral over $\Gamma_{LG}$ in the second equation would cancel out.

5.2.2 Basic definitions

In the following, $\mathcal{T}_h := \mathcal{T}_h(\Omega) := \{\mathcal{K}_i : i = 1, \ldots, N_{el}\}$ denotes a $d$-dimensional, non-overlapping, polytopic partition of $\Omega$ (see [134, Def. 1.12]; with parameter $h$
noting the maximum diameter of an element of the partition) that can be subdivided into $\mathcal{T}_h(\Omega^1)$ and $\mathcal{T}_h(\Omega^g)$ which are partitions of $\Omega^1$ and $\Omega^g$, respectively, and that is for simplicity assumed to be geometrically conformal (in the sense of
[136, Def. 1.55]). All proofs and arguments also hold true for non-geometrically
conformal meshes, but in this case the notation becomes much more technical.

We denote by $\mathcal{F} := \mathcal{F}(\mathcal{T}_h)$ the set of faces, by $\mathcal{F}_I$ the set of interior faces (that do not intersect with $\Gamma_{LG}$), by $\mathcal{F}_E$ the set of exterior faces, and by $\mathcal{F}_T$ the set of faces that belong to $\Gamma_{LG}$. Henceforth, we assume that all $F \in \mathcal{F}_E$ either are elements of $\mathcal{F}_D$ (Dirichlet boundary faces) or of $\mathcal{F}_N$ (Neumann boundary faces) and write $h_F := \text{diam} F$ for the diameter of $F \in \mathcal{F}$. Note that every face of the mesh is an element of one and only one of the following sets: $\mathcal{F}_I$, $\mathcal{F}_T$, $\mathcal{F}_D$, $\mathcal{F}_N$.

Additionally, the sets $\mathcal{F}_I^\alpha$, $\mathcal{F}_D^\alpha$, $\mathcal{F}_N^\alpha$ include all interfaces, Dirichlet boundary
faces, Neumann boundary faces of $\Omega^a$, respectively. No face is allowed to be a member of more than one of these sets.

The test- and ansatz-spaces for our LDG method are defined as the broken polynomial spaces of order at most $k$;

$$
\mathcal{P}^d_k(T_h) := \left\{ v \in L^2(\Omega)^d : v_{\mid K} \text{ is a polynomial of degree at most } k, \forall K \in T_h \right\}.
$$

For an element-wise defined scalar function $w$ and an element-wise vector function $v$ smooth enough to have traces, we define the average $\{|\cdot|\}$ and the jump $[\cdot]$ on $\partial\mathcal{K}_i \cap \partial\mathcal{K}_j$ for neighboring mesh elements $\mathcal{K}_i, \mathcal{K}_j \in T_h, \mathcal{K}_i \neq \mathcal{K}_j$ in the following way:

$$
\|w\| = \frac{1}{2}(w_{\mid \mathcal{K}_i} + w_{\mid \mathcal{K}_j}), \quad [w] = w_{\mid \mathcal{K}_i}v_{\mathcal{K}_i} + w_{\mid \mathcal{K}_j}v_{\mathcal{K}_j},
$$

$$
\|v\| = \frac{1}{2}(v_{\mid \mathcal{K}_i} + v_{\mid \mathcal{K}_j}), \quad [v] = v_{\mid \mathcal{K}_i} \cdot v_{\mathcal{K}_i} + v_{\mid \mathcal{K}_j} \cdot v_{\mathcal{K}_j},
$$

where $v_{\mathcal{K}}$ is defined as the outward unit normal with respect to $\mathcal{K}$. Note, that a jump in a scalar variable is a vector, whereas a jump of a vector is a scalar, and that the jump on $F \in F_E$ with $F \subset \partial\mathcal{K}$ is defined as

$$
[w] = w_{\mid \mathcal{K}}v_{\mathcal{K}}, \quad [v] = v_{\mid \mathcal{K}} \cdot v_{\mathcal{K}}.
$$

### 5.2.3 Spatial discretization

With these definitions we can formulate the semi-discrete problem, where we have to be careful defining numerical fluxes across $\Gamma_{\rm LG}$ since they have to be both locally mass conservative and stabilizing. This is done in the following way for every $\mathcal{K} \in T_h(\Omega)$, every test function $\varphi_i = 1, \ldots, k, \hat{\varphi}_i = 1, \ldots, \hat{k}$, and a.e. $t \in (0, T)$.

Note that $u_h(0)$ is constructed as the element-wise $L^2$-projection of $u_0$, and that $u_h \in \mathcal{P}_k(T_h)$ and $q_h \in \mathcal{P}^d_k(T_h)$, and therefore, we have a different amount of test functions in the following equations, where $\eta$ denotes the penalty parameter:

If $\mathcal{K} \subset \Omega^1$, we have

$$
\int_\mathcal{K} \partial_t u_h \varphi_i \, dx - \sum_{F \in \mathcal{F}_K \cap \mathcal{F}_I} \int_F (\|q_h\| \cdot v_{\mathcal{K}} + \frac{\eta}{h_F} [u_h] \cdot v_{\mathcal{K}}) \varphi_i \, d\sigma
+ \sum_{F \in \mathcal{F}_K \cap \mathcal{F}_T} \int_F (\|q_h\| \cdot v_{\mathcal{K}} + \frac{\eta}{h_F} (u_h^1 - H_{\Gamma_{\rm LG}} u_h^0) \varphi_i) \, d\sigma - \int_\mathcal{K} f \varphi_i \, dx
$$
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\[ + \sum_{F \in T_K \cap F_D} \int_F \left( q_h \cdot \nu_j + \frac{\eta}{h_F} (u_h - u_D) \right) \varphi_i \, d\sigma + \sum_{F \in T_K \cap F_N} \int_F g_N \varphi_i \, d\sigma = 0, \]

and for \( m = 1, \ldots, d \)

\[ + \sum_{F \in T_K \cap F_D} \int_F (\mathbb{q}_h \cdot \nu_j) \varphi_i \, d\sigma + \sum_{F \in T_K \cap F_I} \int_F \mathbb{u}_h \varphi_i (\nu_j) \varphi_j \, d\sigma + \sum_{F \in T_K \cap F_I} \frac{1}{2} \left( \mathbb{u}_h + H^{\Gamma_{LG}} u_h^\epsilon \right) \varphi_i (\nu_j) \varphi_j \, d\sigma + \sum_{F \in T_K \cap F_N} \int_F g_N \varphi_i \, d\sigma = 0. \]

If \( K \subset \Omega^b \), we have

\[ \int_K \partial_i u_h \varphi_i \, dx - \int_K q_h \cdot \nabla \varphi_i \, dx + \sum_{F \in T_K \cap F_I} \left( \int_F (\mathbb{q}_h \cdot \nu_j) \varphi_i + \frac{\eta}{h_F} \mathbb{u}_h \varphi_i (\nu_j) \varphi_j \right) \varphi_i \, d\sigma \]

\[ + \sum_{F \in T_K \cap F_D} \int_F (\mathbb{q}_h \cdot \nu_j) \varphi_i + \frac{\eta}{h_F} (H^{\Gamma_{LG}} u_h^\epsilon - u_h^\epsilon) \varphi_i \, d\sigma - \int_K \mathbb{u}_h \varphi_i \, dx \]

\[ + \sum_{F \in T_K \cap F_I} \left( \int_F q_h \cdot \nu_j + \frac{\eta}{h_F} (u_h - u_D) \right) \varphi_i \, d\sigma + \sum_{F \in T_K \cap F_N} \int_F g_N \varphi_i \, d\sigma = 0, \]

and for \( m = 1, \ldots, d \)

\[ \int_K (D^{-1}(u_h) q_h)_m \varphi_i \, dx - \int_K u_h (\partial_{x_m} \varphi_i) \, dx + \sum_{F \in T_K \cap F_I} \int_F (\mathbb{q}_h \cdot \nu_j)_m \varphi_i \, d\sigma \]

\[ + \sum_{F \in T_K \cap F_D} \int_F (\mathbb{u}_h \varphi_i (\nu_j))_m \, d\sigma + \sum_{F \in T_K \cap F_I} \frac{1}{2} \left( \mathbb{u}_h^\epsilon + u_h^\epsilon \right) \varphi_i \, d\sigma \]

\[ + \sum_{F \in T_K \cap F_N} \int_F u_h \varphi_i \varphi_j \, d\sigma = 0. \]

The **penalty terms** in the first equations ensure the **jump condition** and **local mass conservation** at \( \Gamma_{LG} \) while the **average weighted** \( H^{\Gamma_{LG}} \) in the second equation allows the arguments of Theorem 5.2.13 / [9, Theorem 1] to be carried out on \( \tilde{u} \) and therefore ensures stability of the method.

**Corollary 5.2.3.** The above numerical discretization is consistent with respect to Definition 5.2.2 that is, the above equations hold for a weak solution of (5.1). ▲
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5.2.4 A collection of auxiliary definitions and results

Now, a brief overview of auxiliary definitions and results that are needed for the following analysis is given. The proofs for most of the propositions work analogously to those in [9, pp. 1379–1381]. At first, we define the operator “\( \tilde{\xi} \)” like in (5.2), i.e. for any function \( \xi \) on \( \Omega \)

\[
\tilde{\xi} = \begin{cases} 
\xi & \text{in } (0, T) \times \Omega^1 \\
H_{\Gamma_{G}}^{\xi} & \text{in } (0, T) \times \Omega^8
\end{cases}
\]

and

\[
e_{u} := u_{h} - \pi(u), \quad \theta_{u} := \pi(u) - u, \quad \bar{e}_{u} := \bar{e}_{u}, \quad \bar{\theta}_{u} := \bar{\theta}_{u},
\]

\[
e_{q} := q_{h} - \pi(q), \quad \theta_{q} := \pi(q) - q, \quad \bar{e}_{q} := \bar{e}_{q}, \quad \bar{\theta}_{q} := \bar{\theta}_{q},
\]

where \( \pi \) denotes the \( L^2 \)-projection. Note that \( \pi(u) \in \mathbb{P}_{k}(\mathcal{T}_{h}) \) and \( \pi(q) \in \mathbb{P}_{k}(\mathcal{T}_{h}) \).

**Definition 5.2.4** (Shape and contact regularity). A family of meshes \( (\mathcal{T}_{h})_{h>0} \) is said to be **shape and contact regular** (for short **regular**) if, for all \( h > 0 \), \( \mathcal{T}_{h} \) admits a geometrically conformal, matching simplicial submesh (see [134, Def. 1.37]) \( \widetilde{\mathcal{T}}_{h} \) such that

1. \( (\widetilde{\mathcal{T}}_{h})_{h>0} \) is **shape-regular** in the usual sense of [122], meaning that there is a parameter \( \lambda_{1} > 0 \), independent of \( h \), such that for all \( \tilde{K} \in \widetilde{\mathcal{T}}_{h} \),

\[
\lambda_{1}h_{\tilde{K}} \leq \rho_{\tilde{K}},
\]

where \( \rho_{\tilde{K}} \) is the diameter of the largest ball that can be inscribed in \( \tilde{K} \).

2. there is a constant \( \lambda_{2} > 0 \), independent of \( h \), such that for all \( \mathcal{K} \in \mathcal{T}_{h} \) and for all \( \tilde{K} \in \widetilde{\mathcal{T}}_{h} \) with \( \tilde{K} \subset \mathcal{K} \),

\[
\lambda_{2}h_{\mathcal{K}} \leq h_{\tilde{K}},
\]

\( \triangle \)

For the direct consequences of this definition the reader may consult [134, Section 1.4.1].

**Lemma 5.2.5.** Let \( \mathcal{K} \) and \( \tilde{\mathcal{K}} \) be bounded domains in \( \mathbb{R}^{d} \), and let \( \Phi_{\mathcal{K}} \) be an affine-linear and bijective mapping with \( \Phi_{\mathcal{K}}(\tilde{\mathcal{K}}) = \mathcal{K}, \Phi_{\mathcal{K}}(x) = Bx + b \). For \( k \in \mathbb{N}_{0}, 1 \leq p \leq \infty \) and \( \tilde{u} \in W^{k,p}(\tilde{\mathcal{K}}) \), the following holds:

\( u = \tilde{u} \circ \Phi_{\mathcal{K}}^{-1} \) is in \( W^{k,p}(\mathcal{K}) \) and there is a constant \( C_{\text{traf}} = C_{\text{traf}}(k, p, d) > 0 \) such that

\[
|\tilde{u}|_{W^{k,p}(\tilde{\mathcal{K}})} \leq C_{\text{traf}}h_{\mathcal{K}}^{k}|\det(B)|^{1/p}|u|_{W^{k,p}(\mathcal{K})},
\]
\[ |u|_{W^{k,p}(K)} \leq C_{\text{tr}(1/\rho K)}^k |\det(B)|^{1/p} |u|_{W^{k,p}({\overline{K}}')} \]

with \( \rho K \) defined as in Definition 5.2.4.

\textbf{Proof.} The result is a simple combination of [122, Theorem 15.1] and [145, Theorem 3.27]. \( \square \)

\textbf{Lemma 5.2.6 (Discrete Trace Inequality).} Let \((T_h)\) be a regular mesh sequence with parameters \( \lambda_i, i = 1, 2 \) (as in Definition 5.2.4). Then for all \( h > 0 \), all \( p \in \mathbb{P}_k(T_h) \)

\[ \sum_{F \in T} \|p\|_{L^2(F)} \leq C_{\text{tr}} \sum_{K \in T_h} h_K^{-1/2}\|p\|_{L^2(K)}, \]

where \( C_{\text{tr}} \) only depends on \( \lambda_i, i = 1, 2; d, \) and \( k \). For \( F \) shared by elements \( K_i \) and \( K_j \), the first term in the above inequality is considered to contain both traces:

\[ \|p\|_{L^2(F)} = \|p|_{K_i}\|_{L^2(F)} + \|p|_{K_j}\|_{L^2(F)}. \]

\( \square \)

\textbf{Proof.} This result follows directly from [134, Lemma 1.46] and Definition 5.2.4. \( \square \)

\textbf{Lemma 5.2.7 (Common Trace Inequality).} Let \((T_h)\) be a regular mesh sequence with parameters \( \lambda_i, i = 1, 2 \). Then for all \( h > 0 \), all \( u \in H^{k+1}(\Omega^1 \cup \Omega^2) \), and \( k \in \mathbb{N}_0 \)

\[ \sum_{F \in T} \|\theta_u\|_{L^2(F)} \leq C' \sum_{K \in T_h} h_K^{k+1/2}|u|_{H^{k+1}(K)} \]

where \( C' \) only depends on \( \lambda_i, i = 1, 2; d, \) and \( k \).

\( \square \)

\textbf{Proof.} This is a direct consequence of [134, Lemma 1.49 & Lemma 1.59]. \( \square \)

\textbf{Corollary 5.2.8.} Let \((T_h)_{h>0}\) be a regular mesh sequence with parameters \( \lambda_i, i = 1, 2 \) (as in Definition 5.2.4). Then for all \( h > 0 \), all \( u \in H^{k+1}(\Omega^1 \cup \Omega^2) \), \( q \in H^{k+1}(\Omega^1 \cup \Omega^2)^d \) we have

\[ \sum_{F \in T_i} \|\nabla u\|_{L^2(F)} \leq Ch^{k+1/2}|u|_{H^{k+1}(\Omega)}, \]

\[ \sum_{F \in T_i} \|\theta_q\|_{L^2(F)} \leq Ch^{k+1/2}|q|_{H^{k+1}(\Omega)}, \]

\[ \sum_{F \in T_i} \|\bar{\theta} u\|_{L^2(F)} \leq Ch^{k+1/2}|u|_{H^{k+1}(\Omega)}, \]

\[ \sum_{F \in T_i} \|\nabla q\|_{L^2(F)} \leq Ch^{k+1/2}|q|_{H^{k+1}(\Omega)} \]
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\[
\sum_{F \in \mathcal{T}_E} \| \theta_h \|_{L^2(F)} \leq C h^{k+1/2} |q|_{H^{k+1}(\Omega)} ,
\]

\[
\sum_{F \in \mathcal{T}_E} \| \theta_u \|_{L^2(F)} \leq C h^{k+1/2} |u|_{H^{k+1}(\Omega)} ,
\]

where \( C \) only depends on \( \lambda_i, i = 1, 2; d, k \).

\[\text{Corollary 5.2.9.}\] Let \( \mathcal{T}_h \) be a mesh. For all \( F \in \mathcal{F} \) and all \( v : F \to \mathbb{R}^d \) we have

\[
\| v \cdot \nu \|_{L^2(F)} \leq \sqrt{d} \| v \|_{L^2(F)} .
\]

\[\text{Corollary 5.2.10 (Symmetric Identity).}\] Assume that \( \mathcal{T}_h \) is a mesh of \( \Omega \). Then for every \( \mathbb{R} \)-valued function \( w \) and \( \mathbb{R}^d \)-valued function \( v \) that are defined on each cell of the mesh and smooth enough to have traces, and all \( F \in \mathcal{T}_1 \) we have

\[
\int_F \| w \| \cdot \| v \| \, d\sigma + \int_F \| w \| \cdot \| v \| \, d\sigma = \int_F \| w v \| \, d\sigma .
\]

\[\text{Lemma 5.2.11 (Inverse Identity for polytopic meshes).}\] Let \( \mathcal{T}_h \) be a regular mesh, \( \mathcal{K} \in \mathcal{T}_h \). Then there is a constant \( C_{inv} \) independent of \( h \) such that

\[
|p|^2_{H^1(\mathcal{K})} \leq C_{inv} h^{-2} \| p \|^2_{L^2(\mathcal{K})} , \quad \forall p \in \mathbb{P}_1^k(\mathcal{T}_h) .
\]

\[\text{Proof.}\] See [134, Lemma 1.44].

\[\text{Remark 5.2.12.}\]

1. For any \( w \in \mathbb{P}_k^1(\mathcal{T}_h) \) and \( v \in \mathbb{P}_k^d(\mathcal{T}_h) \), \( (\nabla w) \in \mathbb{P}_k^d(\mathcal{T}_h) \) and \( (\nabla \cdot v) \in \mathbb{P}_k^1(\mathcal{T}_h) \).

2. The following equations and inequalities hold true for \( \alpha = 1, g \):

\[
\int_{\Omega^a} (D^{-1}(u_h)q_h - D^{-1}(u)q) \cdot e_q \, dx
\]

\[
= \int_{\Omega^a} \left[ D^{-1}(u_h)e_q + D^{-1}(u_h)\theta_q + (D^{-1}(u_h) - D^{-1}(u) q) \right] \cdot e_q \, dx ,
\]

and since we have, Remark 5.2.1, Young’s inequality, and the Bramble–Hilbert lemma for any \( \epsilon > 0 \) and some constant \( C > 0 \)

\[
\int_{\Omega^a} (D^{-1}(u_h) - D^{-1}(u)) q \cdot e_q \, dx
\]
\[
\leq \epsilon \| e \|_{L^2(\Omega^*)}^2 + \frac{C}{\epsilon} \| q \|_{L^\infty(\Omega^*)}^2 \left( \| e_u \|_{L^2(\Omega)}^2 + h^{2k+2} |u|_{H^{k+1}(\Omega)}^2 \right).
\]

This needs that \( q \in L^2(0, T; L^\infty(\Omega)^d) \) which is assumed to hold true in the non-linear case. A proof for a more elaborate (but yet similar) result can be found in Lemma 5.4.6.

### 5.2.5 Stability of the method

**Theorem 5.2.13 (Stability of the discrete problem).** Assume that \((u, q)\) satisfy Definition 5.2.2. For every regular, geometrically conformal family of meshes \((T_h)_{h>0}\), all \(\eta, h > 0\) introduced in Section 5.2.3 there is a function \(C\) such that for almost every \(s \in (0, T)\):

\[
\| u_h(s, \cdot) \|_{L^2(\Omega)}^2 + \int_0^s \left[ \left\| \sqrt{D^{-1}(u_h)q_h} \right\|_{L^2(\Omega)}^2 + \sum_{F \in \mathcal{T}_I \cup \mathcal{T}_N \cup \mathcal{T}_D} \frac{\eta}{h_F} \| \left[ u_h \right] \|_{L^2(F)}^2 \right] \, dt \leq C(s). \tag{5.3}
\]

Additionally if \( T < \infty \), we have \( C(s) < \overline{C} \) for some \( \overline{C} \in \mathbb{R} \) and \( s \in [0, T] \).  

**Proof.** We test the equations with \( \tilde{u}_h \) and \( \tilde{q}_h \), respectively, and sum over all \( \mathcal{K} \in \mathcal{T}_h \). This yields

\[
\int_{\Omega} (D^{-1}(u_h)q_h) \cdot \tilde{q}_h \, dx - \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} q_h \cdot \nabla \tilde{u}_h \, dx - \int_{\Omega} f \tilde{u}_h \, dx + \sum_{F \in \mathcal{T}_I} \int_F q_h \cdot \left[ \tilde{u}_h \right] \, d\sigma + \sum_{F \in \mathcal{T}_N} \int_F g_N \tilde{u}_h \, d\sigma + \sum_{F \in \mathcal{T}_D} \int_F (u_h - u_D) \tilde{u}_h \, d\sigma \\
+ \sum_{F \in \mathcal{T}_I} \int_F q_h \cdot v \tilde{u}_h \, d\sigma + \sum_{F \in \mathcal{T}_N} \int_F \| q_h \| \cdot \left[ \tilde{u}_h \right] \, d\sigma + \sum_{F \in \mathcal{T}_D} \int_F \| \tilde{u}_h \|^2 \, d\sigma = 0,
\]

and

\[
\int_{\Omega} (D^{-1}(u_h)q_h) \cdot \tilde{q}_h \, dx - \sum_{\mathcal{K} \in \mathcal{T}_h} \int_{\mathcal{K}} u_h (\nabla \cdot \tilde{q}_h) \, dx \\
+ \sum_{F \in \mathcal{T}_I} \int_F \| u_h \| \cdot \| \tilde{q}_h \| \, d\sigma \\
+ \sum_{F \in \mathcal{T}_N} \int_F u_h \tilde{q}_h \cdot v \, d\sigma + \sum_{F \in \mathcal{T}_D} \int_F u_D \tilde{q}_h \cdot v \, d\sigma
\]
where the terms 2 – 5 on the right hand side of the second equation originate from integration by parts. The sixth term on the right hand side is a combination of terms 6 and 7 on the left hand side. Adding the above equations leads to

\[
\frac{1}{2} \int_{\Omega} \left[ \partial_t (u_h^2) + 2 (D^{-1}(u_h) q_h) \cdot q_h \right] \, dx \\
+ \frac{H_{\text{LG}}}{2} \int_{\Omega^s} \left[ \partial_t (u_h^2) + 2 (D^{-1}(u_h) q_h) \cdot q_h \right] \, dx \\
+ \sum_{F \in \mathcal{F}_I} \frac{\eta}{h_F} \int_F \|u_h\|^2 \, d\sigma + \sum_{F \in \mathcal{F}_s} \frac{H_{\text{LG}} \eta}{h_F} \int_F \|u_h\|^2 \, d\sigma + \sum_{F \in \mathcal{F}_I} \frac{\eta}{h_F} \int_F \|\tilde{u}_h\|^2 \, d\sigma \\
+ \sum_{F \in \mathcal{F}_D} \frac{\eta}{h_F} \int_F \|u_h\|^2 \, d\sigma + H_{\text{LG}} \sum_{F \in \mathcal{F}_D} \frac{\eta}{h_F} \int_F \|u_h\|^2 \, d\sigma \\
= \int_{\Omega} \int f u_h \, dx + H_{\text{LG}} \int_{\Omega^s} f u_h \, dx + \sum_{F \in \mathcal{F}_I} \frac{\eta}{h_F} \int_F u_D u_h \, dx - \sum_{F \in \mathcal{F}_I} \int_F u_D q_h \cdot \nu \, d\sigma \\
+ H_{\text{LG}} \sum_{F \in \mathcal{F}_D} \frac{\eta}{h_F} \int_F u_D u_h \, dx - H_{\text{LG}} \sum_{F \in \mathcal{F}_D} \int_F u_D q_h \cdot \nu \, d\sigma
\]
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\[- \sum_{F \in F_N^d} \int_F g_N u_h \, d\sigma - H^{\Gamma_G} \sum_{F \in F_N^s} \int_F g_N u_h \, d\sigma.\]

Using Young’s and Hölder’s inequalities and the results of Section 5.2.4, we can estimate the $\Xi^a_i$, $a = 1, g$ (similarly to [9, pp. 1382 – 1383]) in the following way:

\[
|\Xi^a_1| \leq \frac{1}{4} \|u_h\|^2_{L^2(\Omega^a)} + \|f\|^2_{L^2(\Omega^a)}
\]

\[
|\Xi^a_2| \leq \frac{1}{2} \sum_{F \in F_D^a} \frac{\eta}{h_F} \|u_h\|^2_{L^2(F)} + \frac{1}{2} \sum_{F \in F_D^s} \frac{\eta}{h_F} \|u_D\|^2_{L^2(F)}
\]

\[
|\Xi^a_3| \leq \frac{1}{2C_D} \|q_h\|^2_{L^2(\Omega^a)} + \sum_{F \in F_D^s} \frac{C_3}{h_F} \|u_D\|^2_{L^2(F)}
\]

\[
|\Xi^a_4| \leq \frac{1}{4} \|u_h\|^2_{L^2(\Omega^a)} + \sum_{F \in F_D^s} \frac{C_4}{h_F} \|g_N\|^2_{L^2(F)}
\]

Here, $C_3$, $C_4$ are constants (only depending on $C_D$, $d$, and $C_N$). Hence

\[
\frac{1}{2} \int_{\Omega^1} [\partial_t (u_h^2) + (D^{-1}(u_h)q_h) \cdot q_h] \, dx + \frac{H^{\Gamma_G}}{2} \int_{\Omega^s} [\partial_t (u_h^2) + (D^{-1}(u_h)q_h) \cdot q_h] \, dx
\]

\[
+ \sum_{F \in F_D^s} \frac{\eta}{h_F} \int_F \|u_h\|^2 \, d\sigma + \sum_{F \in F_D^s} \frac{H^{\Gamma_G} \eta}{h_F} \int_F \|u_h\|^2 \, d\sigma + \sum_{F \in F_D} \frac{\eta}{h_F} \int_F \|\bar{u}_h\|^2 \, d\sigma
\]

\[
+ \frac{1}{2} \sum_{F \in F_D} \frac{\eta}{h_F} \int_F \|u_h\|^2 \, d\sigma + H^{\Gamma_G} \frac{1}{2} \sum_{F \in F_D^s} \frac{\eta}{h_F} \int_F \|u_h\|^2 \, d\sigma
\]

\[
\leq \frac{1}{2} \|u_h\|^2_{L^2(\Omega^1)} + \frac{H^{\Gamma_G}}{2} \|u_h\|^2_{L^2(\Omega^s)} + \|f\|^2_{L^2(\Omega^1)} + H^{\Gamma_G} \|f\|^2_{L^2(\Omega^s)}
\]

\[
+ \sum_{F \in F_D^s} \left( \frac{C_3}{h_F} + \frac{\eta}{2h_F} \right) \|u_D\|^2_{L^2(F)} + H^{\Gamma_G} \sum_{F \in F_D^s} \left( \frac{C_3}{h_F} + \frac{\eta}{2h_F} \right) \|u_D\|^2_{L^2(F)}
\]

\[
+ \sum_{F \in F_D^s} \frac{C_4}{h_F} \|g_N\|^2_{L^2(F)} + H^{\Gamma_G} \sum_{F \in F_D^s} \frac{C_4}{h_F} \|g_N\|^2_{L^2(F)}
\]

and therefore we also have (5.3) (having integrated over time, used Grönwall’s inequality, and multiplied by the factor $2 \max\{H^{\Gamma_G}, (H^{\Gamma_G})^{-1}\}$) with

\[
C(s) = \left( 2 \int_0^s \left[ \|f\|^2_{L^2(\Omega)} + \sum_{F \in F_N^s} \frac{C_4}{h_F} \|g_N\|^2_{L^2(F)} + \sum_{F \in F_D^s} \left( \frac{C_3}{h_F} + \frac{\eta}{2h_F} \right) \|u_D\|^2_{L^2(F)} \right] \, dt \right).
\]

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+ \|u_h(0, \cdot)\|_{L^2(\Omega)}^2 \) \cdot \max\{H_{LG}, (H_{LG})^{-1}\} \exp(s)

This completes the proof. \(\square\)

**Remark 5.2.14.**

- Considering the simplified problem

\[
\begin{cases}
\partial_t \mathbf{u} + \nabla \cdot \mathbf{q} = f & \text{in } (0, T) \times (\Omega^1 \cup \Omega^g), \\
D^{-1}(\mathbf{u})\mathbf{q} + \nabla \mathbf{u} = 0 & \text{in } (0, T) \times (\Omega^1 \cup \Omega^g), \\
\mathbf{u}^1 \cdot \mathbf{v}^1 + \mathbf{q}^6 \cdot \mathbf{v}^6 = 0 & \text{in } (0, T) \times \Gamma_{LG}, \\
\mathbf{q} \cdot \mathbf{v} = g_N & \text{on } (0, T) \times \Gamma_N, \\
\mathbf{u} = \mathbf{u}_D & \text{on } (0, T) \times \Gamma_D, \\
\mathbf{u}(0, \mathbf{x}) = \mathbf{u}_0(\mathbf{x}) & \text{in } \Omega^1 \cup \Omega^g
\end{cases}
\]

implies \( \Xi_1^a = \Xi_4^a = 0 \), therefore the right hand side of (5.4) simplifies to

\[
\leq \sum_{F \in \mathcal{T}_D} \left( \frac{C_3}{h_F} + \frac{\eta}{2h_F} \right) \|u_D\|_{L^2(F)}^2 + H_{LG} \sum_{F \in \mathcal{T}_D} \left( \frac{C_3}{h_F} + \frac{\eta}{2h_F} \right) \|u_D\|_{L^2(F)}^2
\]

i.e., the semi-discrete LDG solution is unconditionally and uniformly stable if \( u_D \equiv 0 \).

- The proof can also be performed for an arbitrary (but finite) number of subdomains \( \Omega^{\alpha_i} \) if the constants \( H_{\Gamma^{\alpha_i, \alpha_j}} \) (for all subdomains \( \alpha_i, \alpha_j \) touching each other) satisfy consistency conditions that allow the "\( \widetilde{\cdot} \)" operator to be well defined.

- In the case that \( H_{LG} : L^2((0, T) \times \Omega) \rightarrow [a, b] \) is a function and strongly Lipschitz (see Remark 5.2.1) with \( a, b > 0 \), the above proof still works with slight modifications.

### 5.2.6 Convergence order estimates

**Theorem 5.2.15.** Assume that \((\mathbf{u}, \mathbf{q})\) is \((\hat{k} + 1, k + 1)\)-regular. For every regular, geometrically conformal family of meshes \((\mathcal{T}_h)_{h > 0}, \eta > 0, |\hat{k} - k| \leq 1\), the solution of the algorithm of Section 5.2.3 \((u_h, q_h)\) converges for almost every \( s \in (0, T) \) with order min\{\(\hat{k}, k + 1\)\} to \((\mathbf{u}, \mathbf{q})\) in the following sense:

\[
\|e_u(s, \cdot)\|_{L^2(\Omega)}^2 + \int_0^s \left( \|e_q\|_{L^2(\Omega)}^2 + \sum_{F \in \mathcal{T}(\Omega) \cup \mathcal{T}_D} \frac{\eta}{h_F} \|\tilde{\iota}_F \|_{L^2(F)}^2 \right) dt \leq Ch^{2 \min\{\hat{k}, k+1\}}
\]
for some constant $C > 0$ independent of $h$. \hfill \blacksquare

**Remark 5.2.16.** As a direct consequence of Theorem 5.2.15 we obtain

$$
\| (u_h - u)(s,) \|_{L^2(\Omega)} + \int_0^s \| q_h - q \|_{L^2(\Omega')} \, dt \leq C_h \min(\hat{k}, k+1) \quad \text{for } s \in (0, T).
$$

**Proof.** We use the consistency of the numerical scheme, sum over all $K \in T_h$, test the equations with $\tilde{e}_u$ and $\tilde{e}_q$, respectively, subtract the corresponding equations from one another, and use the fact that $u_h - u = e_u + \theta_u$, $q_h - q = e_q + \theta_q$. This yields

$$
\int_\Omega \partial_t (e_u + \theta_u) \tilde{e}_u \, dx - \sum_{K \in T_h} \int_K (e_q + \theta_q) \cdot \nabla \tilde{e}_u \, dx + \sum_{F \in T_D} \int_F (e_q + \theta_q) \cdot \nu \tilde{e}_u \, d\sigma \\
+ \sum_{F \in T_I} \int_F \| e_q + \theta_q \| \cdot \| \tilde{e}_u \| \, d\sigma + \sum_{F \in T_D} \frac{\eta}{h_F} \int_F \| \tilde{e}_u + \theta_u \| \cdot \| \tilde{e}_u \| \, d\sigma \\
+ \sum_{F \in T_I} \int_F \| e_q + \theta_q \| \cdot \| \tilde{e}_u \| \, d\sigma + \sum_{F \in T_I} \frac{\eta}{h_F} \int_F \| \tilde{e}_u + \theta_u \| \cdot \| \tilde{e}_u \| \, d\sigma = 0,
$$

$$
\int_\Omega \left( D^{-1}(u_h) q_h - D^{-1}(u) q \right) \cdot \tilde{e}_q \, dx - \sum_{K \in T_h} \int_K (e_u + \theta_u) (\nabla \cdot \tilde{e}_q) \, dx \\
+ \sum_{F \in T_I} \int_F (e_u + \theta_u) \tilde{e}_q \cdot \nu \, d\sigma + \sum_{F \in T_I} \int_F \| e_u + \theta_u \| \| \tilde{e}_q \| \, d\sigma \\
+ \sum_{F \in T_I} \int_F \| \tilde{e}_u + \theta_u \| \| e_q \| \, d\sigma
$$

$$
= \int_\Omega \left( D^{-1}(u_h) q_h - D^{-1}(u) q \right) \cdot \tilde{e}_q \, dx + \sum_{K \in T_h} \int_K \nabla \tilde{e}_u \cdot e_q \, dx - \sum_{F \in T_D \cup T_N} \int_F \tilde{e}_u e_q \cdot \nu \, d\sigma \\
- \sum_{F \in T_I} \int_F \| \tilde{e}_u e_q \| \, d\sigma - \sum_{F \in T_I} \int_F \| \tilde{e}_u e_q \| \, d\sigma + \sum_{F \in T_I} \int_F (e_u + \theta_u) \tilde{e}_q \cdot \nu \, d\sigma \\
+ \sum_{F \in T_I} \int_F \| e_u + \theta_u \| \| \tilde{e}_q \| \, d\sigma + \sum_{F \in T_I} \int_F \| \tilde{e}_u + \theta_u \| \| e_q \| \, d\sigma = 0.
$$

Note that $\theta_q$ and $\theta_u$ can be omitted since they are $L^2$-orthogonal on polynomials of degree $\hat{k}$ and $k$, respectively. This is ensured by Remark 5.2.12 and executed in the second equation. In the following, we omit the volume terms $\partial_t \theta_u$, $\theta_q$ of the
first equation without mentioning this explicitly. Adding both equations, simple
algebraic manipulations, and Remark 5.2.12 lead to the following equation:

\[
\frac{1}{2} \int_{\Omega} \left[ \partial_t(e_u)^2 + D^{-1}(u_h)e_q \cdot e_q \right] \, dx + \frac{H_{\text{LG}}}{2} \int_{Q^k} \left[ \partial_t(e_u)^2 + D^{-1}(u_h)e_q \cdot e_q \right] \, dx \\
+ \sum_{F \in F_1^D} \frac{\eta}{h_F} \int_F \|e_u\|^2 \, d\sigma + H_{\text{LG}} \sum_{F \in F_1^D} \frac{\eta}{h_F} \int_F \|e_u\|^2 \, d\sigma + \sum_{F \in F_1^D} \frac{\eta}{h_F} \int_F \|\bar{e}_u\|^2 \, d\sigma \\
+ \sum_{F \in F_1^D} \frac{\eta}{h_F} \int_F \|e_u\|^2 \, d\sigma + H_{\text{LG}} \sum_{F \in F_1^D} \frac{\eta}{h_F} \int_F \|e_u\|^2 \, d\sigma \\
= - \int_{\Omega} (D^{-1}(u_h)\theta_q) \cdot e_q \, dx - H_{\text{LG}} \int_{Q^k} (D^{-1}(u_h)\theta_q) \cdot e_q \, dx - \sum_{F \in F_1^D} \int_F \theta_q \cdot v e_u \, d\sigma \\
=: \mathbb{E}_1^1 \\
- H_{\text{LG}} \sum_{F \in F_1^D} \int_F \theta_q \cdot v e_u \, d\sigma - \sum_{F \in F_1^D} \int_F \theta_q \cdot \|e_u\| \, d\sigma - \sum_{F \in F_1^D} \int_F \theta_q \cdot \|\bar{e}_u\| \, d\sigma \\
=: \mathbb{E}_2^1 \\
- H_{\text{LG}} \sum_{F \in F_1^D} \int_F \theta_q \cdot \|e_u\| \, d\sigma - \sum_{F \in F_1^D} \int_F \theta_q \cdot \|\bar{e}_u\| \, d\sigma - H_{\text{LG}} \sum_{F \in F_1^N} \int_F \theta_u e_q \cdot v \, d\sigma \\
=: \mathbb{E}_2^2 \\
- \sum_{F \in F_1^N} \int_F \|\bar{\theta}_u\| \cdot \|e_q\| \, d\sigma - \sum_{F \in F_1^N} \int_F \|\bar{\theta}_u\| \cdot \|\bar{e}_u\| \, d\sigma - H_{\text{LG}} \sum_{F \in F_1^N} \int_F \|\theta_u\| \cdot \|e_q\| \, d\sigma \\
=: \mathbb{E}_3^N \\
- \sum_{F \in F_1^N} \int_F \|\bar{\theta}_u\| \cdot \|e_q\| \, d\sigma - \sum_{F \in F_1^N} \int_F \|\bar{\theta}_u\| \cdot \|\bar{e}_u\| \, d\sigma - H_{\text{LG}} \sum_{F \in F_1^N} \int_F \|\bar{\theta}_u\| \cdot \|\bar{e}_u\| \, d\sigma \\
=: \mathbb{E}_3^l \\
- \sum_{F \in F_1^N} \int_F \|\bar{\theta}_u\| \cdot \|e_q\| \, d\sigma - \sum_{F \in F_1^N} \int_F \|\bar{\theta}_u\| \cdot \|\bar{e}_u\| \, d\sigma - H_{\text{LG}} \sum_{F \in F_1^N} \int_F \|\bar{\theta}_u\| \cdot \|\bar{e}_u\| \, d\sigma \\
=: \mathbb{E}_4^N \\
- \sum_{F \in F_1^N} \int_F \|\bar{\theta}_u\| \cdot \|e_q\| \, d\sigma - \sum_{F \in F_1^N} \int_F \|\bar{\theta}_u\| \cdot \|\bar{e}_u\| \, d\sigma \\
=: \mathbb{E}_4^l \\
\]
\[- \int_{\Omega^l} (D^{-1}(u_h) - D^{-1}(u)) \cdot q \cdot e_q \, dx \]

\[= : \Xi^l \]

\[- H^{fg \alpha} \int_{\Omega^g} (D^{-1}(u_h) - D^{-1}(u)) \cdot q \cdot e_q \, dx \]

\[= : \Xi^g \]

Now, we are able to estimate the $\Xi$s using Young’s and Hölder’s inequalities, the Bramble–Hilbert lemma, well-known properties of the $L^2$-projection, and the results of Section 5.2.4. Very similar estimates are performed in [9, pp. 1387 – 1388] in great detail.

\[|\Xi_{1,a}^a| \leq \sum_{K \in T_h} \|e_q\|_{L^2(K)^d} \|D^{-1}\|_{L^\infty(K)} \|\theta_q\|_{L^2(K)^d} \leq \frac{1}{8C_D} \|e_q\|_{L^2(Q)^d}^2 + C_1^a h^{2k+2} \|q\|_{H^{k+1}(Q)^d}^2, \]

\[|\Xi_{2,a}^a,\beta| \leq \frac{1}{4} \sum_{F \in T_h} \frac{\eta}{h_F} \|\tilde{e}_u\|_{L^2(F)^d}^2 + \frac{C_2^a}{\eta} h^{2k+2} \|q\|_{H^{k+1}(Q)^d}^2, \]

\[|\Xi_{2,\alpha}^f| \leq \frac{1}{4} \sum_{F \in T_h} \frac{\eta}{h_F} \|\tilde{e}_u\|_{L^2(F)^d}^2 + \frac{C_2^f}{\eta} h^{2k+2} \|q\|_{H^{k+1}(Q)^d}^2, \]

\[|\Xi_{3,a}^a,\beta| \leq \frac{1}{8C_D} \|e_q\|_{L^2(Q)^d}^2 + C_3^a h^{2k} \|u\|_{H^{k+1}(Q)}^2, \]

\[|\Xi_{3,a}^f| \leq \frac{1}{4} \sum_{F \in T_h} \frac{\eta}{h_F} \|\tilde{e}_u\|_{L^2(F)^d}^2 + C_3^f h^{2k} \|u\|_{H^{k+1}(Q)}^2, \]

\[|\Xi_{3,\alpha}^f| \leq \frac{1}{4} \sum_{F \in T_h} \frac{\eta}{h_F} \|\tilde{e}_u\|_{L^2(F)^d}^2 + C_3^f h^{2k} \|u\|_{H^{k+1}(Q)}^2, \]

\[|\Xi_{4,a}^a| \leq \frac{1}{8C_D} \|e_q\|_{L^2(Q)^d}^2 + C_4^a \|q\|_{L^\infty(Q)^d}^2 \left( \|e_u\|_{L^2(Q)}^2 + h^{2k+2} \|u\|_{H^{k+1}(Q)}^2 \right), \]

\[|\Xi_{4,f}^f| \leq \frac{1}{4} \sum_{F \in T_h} \frac{\eta}{h_F} \|\tilde{e}_u\|_{L^2(F)^d}^2 + C_4^f \eta h^{2k} \left( \|e_u\|_{L^2(Q)}^2 + h^{2k+2} \|u\|_{H^{k+1}(Q)}^2 \right), \]

\[|\Xi_{5,a}^g| \leq \frac{1}{8C_D} \|e_q\|_{L^2(Q)^d}^2 + C_5^g \|q\|_{L^\infty(Q)^d}^2 \left( \|e_u\|_{L^2(Q)}^2 + h^{2k+2} \|u\|_{H^{k+1}(Q)}^2 \right) \]

Recombining the above results and simple algebraic manipulations lead to

\[\partial_t \|e_u\|_{L^2(Q)}^2 + \sqrt{D^{-1}(u_h) e_q} \left( \|e_u\|_{L^2(Q)}^2 + \sum_{F \in F_h} \frac{\eta}{h_F} \|\tilde{e}_u\|_{L^2(F)}^2 \right) \]
\[ \leq 2 \max \left\{ H^{\Gamma_{\text{LG}}}, \frac{1}{H^{\Gamma_{\text{LG}}}} \right\} \left[ C_{1,2} h^{2k+2} \| q \|^2_{H^{k+1}(\Omega)^d} + C_{3,4} h^{2k} \| u \|^2_{H^{k+1}(\Omega)} \right. \\
+ C_5 \| q \|_{L^\infty(\Omega)^d} \| e_u \|^2_{L^2(\Omega)} + C_5 \| q \|^2_{L^\infty(\Omega)^d} h^{2k+2} \| u \|^2_{H^{k+1}(\Omega)} \right], \quad (5.6) \]

where \( C_{i,j} \) is a recombination of the respective constants in the above estimates (now possibly depending on \( \eta \)). Having integrated with respect to time Grönwall’s inequality yields

\[ \| e_u(s, \cdot) \|^2_{L^2(\Omega)} + \int_0^s \left( \| \sqrt{D^{-1}(u_t)} e_q \|^2_{L^2(\Omega)^d} + \sum_{F \in \mathcal{F}_I \cup \mathcal{F}_T \cup \mathcal{F}_D} \frac{\eta}{h} \| \bar{e}_u \|^2_{L^2(F)} \right) \, dt \]

\[ \leq 2 \max \left\{ H^{\Gamma_{\text{LG}}}, \frac{1}{H^{\Gamma_{\text{LG}}}} \right\} \left[ C_{1,2} h^{2k+2} \int_0^s \| q \|^2_{H^{k+1}(\Omega)^d} \, dt + C_{3,4} h^{2k} \int_0^s \| u \|^2_{H^{k+1}(\Omega)} \, dt \right. \\
+ C_5 \| q \|^2_{L^\infty(\Omega)^d} h^{2k+2} \| u \|^2_{H^{k+1}(\Omega)} \left. \exp \left( 2 \max \left\{ H^{\Gamma_{\text{LG}}}, \frac{1}{H^{\Gamma_{\text{LG}}}} \right\} C_5 \int_0^s \| q \|^2_{L^\infty(\Omega)^d} \, dt \right) \right] \]

At last, we have to take the square root of both sides of the inequality, and use triangle inequality and \( \| \theta_u \|_{L^2(\Omega)} \leq C h^{k+1} \), \( \| \theta_q \|_{L^2(\Omega)} \leq C h^{k+1} \) to obtain the result. \( \square \)

**Remark 5.2.17.**

- If \( D \) is independent of the solution \( u \), \( \mathcal{E}_0^2 = 0 \) and therefore the right hand side of (5.6) simplifies to

\[ \leq 2 \max \left\{ H^{\Gamma_{\text{LG}}}, \frac{1}{H^{\Gamma_{\text{LG}}}} \right\} \left[ C_{1,2} h^{2k+2} \| q \|^2_{H^{k+1}(\Omega)^d} + C_{3,4} h^{2k} \| u \|^2_{H^{k+1}(\Omega)} \right], \]

and Grönwall’s inequality could be skipped in the above proof leading to the following right hand side in (5.7):

\[ \leq 2 \max \left\{ H^{\Gamma_{\text{LG}}}, \frac{1}{H^{\Gamma_{\text{LG}}}} \right\} \int_0^s \left[ C_{1,2} h^{2k+2} \| q \|^2_{H^{k+1}(\Omega)^d} + C_{3,4} h^{2k} \| u \|^2_{H^{k+1}(\Omega)} \right] \, dt, \]

i.e. to an estimate without an exponential term with respect to time.

- The proof can also be performed for an arbitrary (but finite) number of subdomains \( \Omega^{(g)} \) if the constants \( H^{\Gamma_{ai,aj}} \) (for all subdomains \( \alpha_i, \alpha_j \) touching each other) satisfy consistency conditions that allow the “\( \bar{\cdot} \)" operator to be well defined.

- In the case that \( H^{\Gamma_{\text{LG}}} : L^2((0, T) \times \Omega) \to [a, b] \) is a function and strongly Lipschitz (see Remark 5.2.1) with \( a, b > 0 \), the above proof does not work out, since the operator “\( \bar{\cdot} \)" cannot be shifted from the test function to \( e_u + \theta_u \) anymore.
5.2.7 Numerical results

<table>
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<th>$|u_h - u|$</th>
<th>EOC</th>
<th>$|q_h - q|$</th>
<th>EOC</th>
</tr>
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</tr>
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<td>6.57E+0</td>
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</table>

Table 5.1: Convergence results for approximation by $P^0 - P^0$ elements.

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<th>$|u_h - u|$</th>
<th>EOC</th>
<th>$|q_h - q|$</th>
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</table>

Table 5.2: Convergence results for $P^1 - P^1$ and $P^1 - P^0$ approximations.

In this section, numerical results illustrating the performance of the method are presented. To do so, we define the following test example with known solution:

\[
T = 1, \quad \Delta t = 10^{-4}, \quad \eta = 10, \\
\Omega^1 = (0, 10) \times (0, 5), \quad \Omega^8 = (0, 10) \times (5, 10), \\
H_{l,c}^{1,0} = 10, \\
D = \begin{cases} 
0.1 & \text{if } x_2 < 5, \\
1 & \text{otherwise},
\end{cases}
\]
5.2 A LDG scheme for Darcy’s equation including jump conditions

\[ i \quad h \quad \| u_h - u \| \quad \text{EOC} \quad \| q_h - q \| \quad \text{EOC} \]
\[
\begin{array}{cccccc}
1 & 7.071 & 4.04E+1 & -- & 6.89E+0 & -- \\
2 & 3.535 & 2.96E+1 & 0.45 & 6.17E+0 & 0.15 \\
3 & 1.767 & 2.51E+1 & 0.23 & 5.09E+0 & 0.27 \\
4 & 0.883 & 1.39E+1 & 0.85 & 2.94E+0 & 0.79 \\
5 & 0.441 & 4.99E+0 & 1.48 & 1.22E+0 & 1.26 \\
6 & 0.221 & 1.42E+0 & 1.80 & 4.57E-1 & 1.41 \\
7 & 0.110 & 9.63E-2 & 1.93 & 1.81E-1 & 1.33 \\
8 & 0.055 & 2.57E-2 & 1.90 & 8.06E-2 & 1.16 \\
9 & 0.027 & 2.57E-2 & 1.90 & 3.87E-2 & 1.05 \\
\end{array}
\]

Table 5.3: Convergence results for approximation by \( P^1 \) – \( P^2 \) elements.

\[
\begin{array}{cccccc}
\| u_h - u \| & \| q_h - q \| & \text{EOC} & \| u_h - u \| & \| q_h - q \| & \text{EOC} \\
1 & 3.34E+1 & -- & 6.84E+0 & -- & 3.33E+1 & -- \\
2 & 1.10E+1 & 1.59 & 3.72E+0 & 0.87 & 1.10E+1 & 1.59 \\
3 & 2.27E+0 & 2.28 & 1.42E+0 & 1.38 & 2.26E+0 & 2.28 \\
4 & 3.10E-1 & 2.87 & 4.02E-1 & 1.82 & 3.08E-1 & 2.87 \\
5 & 3.35E-2 & 3.20 & 8.88E-2 & 2.17 & 3.24E-2 & 3.25 \\
6 & 5.10E-3 & 2.71 & 1.83E-2 & 2.27 & 5.09E-3 & 2.66 \\
7 & 3.73E-3 & 0.45 & 4.16E-3 & 2.14 & 3.73E-3 & 0.44 \\
\end{array}
\]

Table 5.4: Convergence results for \( P^2 - P^2 \) and \( P^2 - P^1 \) approximations.

\[
u = \begin{cases} 
10 \cos(x_1 + t) \cos(x_2 + t) & \text{if } x_2 < 5, \\
\cos(x_1 + t) \cos(x_2 + t) & \text{otherwise.}
\end{cases}
\]

The upper and lower boundaries are Neumann boundaries, while the left and right boundaries are supposed to be of Dirichlet-type. The right hand side \( f \) and boundary conditions \( u_0, u_D, \) and \( g_N \) are chosen appropriately. We discretize \( \Omega = \Omega^I \cup \Omega^g \) by \( 2^i \times 2^i \) squares (where \( i \) denotes the number of refinements steps) and use ansatz functions \( P^k \) – \( P^k \) on each element. This means, that \( u \) is approximated by polynomials of degree at most \( \tilde{k} \) while \( q \)'s components are approximated by polynomials of degree at most \( k \). Time is discretized using an implicit Euler scheme with constant time-step size \( \Delta t \) and the numerical quadrature is performed using tensor-products of Gaussian quadrature rules being exact for polynomials of degree at most 3, 5, 7, respectively. The results can be found in the Tables 5.1 – 5.4 depicting the \( L^2 \)-errors of the primary and the
flux unknowns and the experimental orders of convergence (EOC). They have been computed using M++ [43].

We can see that our error analysis is sharp for the flux variable $q$, but the primary unknown $u$ tends to have an even higher order of convergence than it could be shown with our analysis. Additionally, we can see that the results in Table 5.2 and Table 5.3 (Table 5.4, respectively) are very similar. This fits perfectly to our analysis since $1 = \min\{1, 1 + 1\} = \min\{1, 2 + 1\} = \min\{1, 0 + 1\}$ $(\min\{2, 2 + 1\} = 2 = \min\{2, 1 + 1\})$, and for that reason all orders of convergence should be equal.

The last lines in Table 5.4 show a suboptimal order of convergence, due to the time-stepping error. Thus, using $\Delta t = 10^{-5}$ for $h = 0.110$ gives errors of 5.0721E-4 and 5.0656E-4 for $u$, and 4.1139E-3 and 4.5048E-3 for $q$, respectively. This restores the full orders of convergence of the scheme.

Our numerical results indicate that the best choice for the method is $\hat{k} = k + 1$, since this minimizes the computational costs and gives an optimal order of convergence.

5.3 An application of the LDG method with different approximation spaces on non-linear advection–diffusion equations

In this study we extend to advection–diffusion problems the work on differing order LDG discretizations introduced in [10] and above for the Darcy equation. Although many well-known results exist for LDG schemes [117], investigations involving differing orders for the state and the flux unknowns are rare (a notable exception is [131]). In this section, the state unknown is approximated by polynomials of order $k + 1$ whereas the flux uses order $k$ — a combination exactly opposite to the choice made in [131], again (and similar to the above section); other major differences are that our scheme needs no reconstructions and has far fewer degrees of freedom in multiple dimensions. By employing classical DG analysis techniques, sharp error estimates for the method are obtained.

Consider an instationary advection–diffusion problem on a bounded, non-degenerated Lipschitz polytope $\Omega \subset \mathbb{R}^d$. We assume $\partial \Omega$ to be disjointly subdivided into the Dirichlet $\Gamma_D$, Neumann $\Gamma_N$, and flux $\Gamma_F$ boundaries with $\nu$ denoting the outward unit normal. We also assume $\nu \cdot \nu \leq 0$ on flux and Dirichlet boundary faces and $\nu \cdot \nu \geq 0$ on Neumann boundaries. The problem (in mixed form) for $f \in L^2(0, T; L^2(\Omega))$, $D^{-1} (u) \in L^\infty(0, T; W^1,\infty(\Omega)^d,d)$ strongly Lipschitz and uniformly symmetric positive definite, $u_D, g_N, g_F \in L^2(0, T; H^1(\Omega))$, and
5.3 An application on non-linear advection–diffusion equations

\[ v \in L^\infty(0, T; W^{1, \infty}(\Omega)^d) \] (like in Section 5.2) is given as follows:

\[
\begin{aligned}
& \partial_t u + \nabla \cdot (v u + q) = f \quad \text{in} \quad (0, T) \times \Omega, \\
& D^{-1}(u) q + \nabla u = 0 \quad \text{in} \quad (0, T) \times \Omega, \\
& (v u + q) \cdot \nabla \psi = g_F \quad \text{on} \quad (0, T) \times \Gamma_F, \\
& q \cdot \nabla \psi = g_N \quad \text{on} \quad (0, T) \times \Gamma_N, \\
& u = u_D \quad \text{on} \quad (0, T) \times \Gamma_D, \\
& u(0, x) = u_0(x) \quad \text{in} \quad \Omega.
\end{aligned}
\] (5.8)

5.3.1 Formulation of the LDG scheme

Note that \( u_h(0) \) is obtained as the element-wise \( L^2 \)-projection of \( u_0 \) and that \( u_h \in F_k(T_h) \), whereas \( q_h \) belongs to \( \mathbb{P}^d(T_h) \) resulting in differing test spaces for (5.9) and (5.10):

\[
\int_{\Omega} \partial_t u_h \varphi \, dx + \mathcal{A}(u_h, \varphi) + \mathcal{B}_u(q_h, \varphi) + \Lambda(u_h, \varphi) = \int_{\Omega} f \varphi \, dx - \int_{\Gamma_F} g_F \varphi \, d\sigma,
\] (5.9)

\[
\int_{\Omega} (D^{-1}(u_h)q_h)_m \psi \, dx + \mathcal{B}_q(u_h, \psi) = 0,
\] (5.10)

where forms \( \mathcal{A}(\cdot, \cdot), \mathcal{B}_u(\cdot, \cdot), \mathcal{B}_q(\cdot, \cdot), \Lambda(\cdot, \cdot) \) are defined as

\[
\mathcal{A}(u_h, \varphi) := \sum_{F \in T_h \cup F_N} \int_F v(u_h)_T \cdot \| \varphi \| \, d\sigma + \sum_{F \in F_D} \int_F v u_D \cdot \| \varphi \| \, d\sigma
\]

\[
- \sum_{K \in T_h} \int_K v u_h \cdot \nabla \varphi \, dx,
\]

\[
\mathcal{B}_u(q_h, \varphi) := \sum_{F \in T_h \cup F_N} \int_F \| q_h \| \cdot \| \varphi \| \, d\sigma + \sum_{F \in F_N} \int_F g_N \varphi \, d\sigma - \sum_{K \in T_h} \int_K q_h \cdot \nabla \varphi \, dx,
\]

\[
\mathcal{B}_q(u_h, \psi) := \sum_{F \in F \setminus F_D} \int_F \| u_h \| \cdot \| \psi \| \, d\sigma + \sum_{F \in F_D} \int_F u_D \psi \, d\sigma - \sum_{K \in T_h} \int_K u_h \nabla \cdot \psi \, dx,
\]

\[
\Lambda(u_h, \varphi) := \sum_{F \in T_h} \frac{\eta}{h_F} \int_F \| u_h \| \cdot \| \varphi \| \, d\sigma + \sum_{F \in F_D} \frac{\eta}{h_F} \int_F (u_h - u_D) \varphi \, d\sigma,
\]

and the upwind flux is defined as

\[
v(w)_T := \begin{cases} v w \big|_{K_t}, & v \cdot v_{K_t} \geq 0, \\ v w \big|_{\Omega \setminus K_t}, & \text{otherwise,} \end{cases} \quad v(w)_T := v w
\]
on internal and external faces, respectively.
5.3.2 Stability and error analysis

The stability and error analysis in this section is an extension to advection–diffusion problems of the results presented in Theorem 5.2.13 / [10, Theorem 4.9] and Theorem 5.2.15 / [10, Theorem 4.11], thus only the advection form \( \mathcal{A}(\cdot, \cdot) \) is treated here. Flux boundary faces used in (5.8) and missing in Section 5.2 / [10] pose no difficulties and will get no further notice.

**Theorem 5.3.1 (Stability of the semi-discrete problem).** For every regular, geometrically conformal family of meshes \((\mathcal{T}_h)_{h>0}\) and any \(\eta > 0\), there exists a function \(C\) such that for a.e. \(s \in (0, T)\):

\[
\|u_h(s, \cdot)\|^2_{L^2(\Omega)} + \int_0^s \left[ \|\sqrt{D^{-1}(u_h)}q_h\|^2_{L^2(\Omega)} + \sum_{F \in \mathcal{T}_h \cup \mathcal{T}_D} \frac{\eta}{h_F} \|\|u_h\||^2_{L^2(F)} \right] \, dt \leq C(s).
\]

Additionally, if \(T < \infty\), there exists some \(\overline{C} \in \mathbb{R}\) s.t. \(C(s) < \overline{C}, \forall s \in [0, T]\).

**Proof.** We set \(\psi := u_h\) and \(\psi := q_h\) in (5.9)–(5.10) and integrate by parts. Using Theorem 5.2.13 for the *advection term*, we consider advection form \(\mathcal{A}(\cdot, \cdot)\)

\[
\mathcal{A}(u_h, u_h) = \frac{1}{2} \int_\Omega (\nabla \cdot v) u_h^2 \, dx - \frac{1}{2} \sum_{F \in \mathcal{T}_h \cup \mathcal{T}_D} \int_F v \cdot v u_h^2 \, d\sigma + \sum_{F \in \mathcal{T}_D} \int_F v u_D \cdot v u_h \, d\sigma
\]

\[
\quad + \sum_{F \in \mathcal{T}_h \cup \mathcal{T}_N} \int_F v \cdot \left( (u_h)^1 \|u_h\| - \frac{1}{2} \|u_h^2\| \right) \, d\sigma
\]

\[
= \frac{1}{2} \int_\Omega (\nabla \cdot v) u_h^2 \, dx + \frac{1}{2} \sum_{F \in \mathcal{T}_D} \int_F |v \cdot v| \|u_h\|^2 \, d\sigma + \sum_{F \in \mathcal{T}_D} \int_F v u_D \cdot v u_h \, d\sigma.
\]

The 2nd term above is a non-negative left-hand-side term; as for the remainder:

\[
\frac{1}{2} \int_\Omega (\nabla \cdot v) u_h^2 \, dx \leq \frac{1}{2} \|\nabla \cdot v\|_{L^\infty(\Omega)} \|u_h\|^2_{L^2(\Omega)},
\]

\[
\sum_{F \in \mathcal{T}_D} \int_F v u_D \cdot v u_h \, d\sigma \leq \|u_h\|^2_{L^2(\Omega)} + C\|v\|_{L^\infty(\mathcal{T}_D)} \sum_{F \in \mathcal{T}_D} h_F^{-1}\|u_D\|^2_{L^2(F)}.
\]

The result follows by combining the above with Theorem 5.2.13 or similar estimates in [1, 9] and applying Grönwall’s lemma.

**Theorem 5.3.2.** For \((u, q)\) \((\hat{k} + 1, k + 1)\)-regular with \(|\hat{k} - k| \leq 1\), every regular, geometrically conformal family of meshes \((\mathcal{T}_h)_{h>0}\), and any \(\eta > 0\), the solution \((u_h, q_h)\) of (5.9)–(5.10) converges to \((u, q)\) for a.e. \(s \in (0, T)\) with order \(min\{\hat{k}, k+1\}:

\[
\|e_u(s, \cdot)\|^2_{L^2(\Omega)} + \int_0^s \left\{ \|e_q\|^2_{L^2(\Omega)} + \sum_{F \in \mathcal{T}_h \cup \mathcal{T}_D} \frac{\eta}{h_F} \|\|e_u\||^2_{L^2(F)} \right\} \, dt \leq Ch^{2 \min\{\hat{k}, k+1\}}
\]

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Remark 5.3.3. As a direct consequence of Theorem 5.3.2 we obtain
\[\|(u_h - u)(s, \cdot)\|_{L^2(\Omega)} + \int_0^s \|q_h - q\|_{L^2(\Omega)} \, dt \leq C h^{\min(k, k+1)}, \quad \text{for a.e. } s \in (0, T).\]

Proof. Setting \(\varphi := e_u\) and \(\psi := e_q\) in (5.9)–(5.10) and using once again Theorem 5.2.15 for the diffusion term, we consider the advection part here. First, note that
\[\int_{\Omega} v e_u \cdot \nabla e_u \, dx = \frac{1}{2} \left( \int_{\Omega} (\nabla \cdot v) e_u^2 \, dx - \sum_{F \in \mathcal{F}} \int_F v \cdot \|e_u^2\| \, d\sigma \right).\]

\[\mathcal{A}(u_h, e_u) - \mathcal{A}(u, e_u) = \sum_{F \in \mathcal{F}\cup\mathcal{F}_N} \int_F v ((e_u + \theta_u)\|e_u\| \, d\sigma - \sum_{K \in h} \int_K v e_u \cdot \nabla e_u \, dx\]
\[= \frac{1}{2} \sum_{F \in \mathcal{F}\cup\mathcal{F}_N} \int_F |v \cdot v| \|e_u\|^2 \, d\sigma + \sum_{F \in \mathcal{F}\cup\mathcal{F}_N} \int_F v \theta_u \cdot \|e_u\| \, d\sigma\]
\[\Xi_1\]
\[\Xi_2\]
\[\Xi_3\]

Using our auxiliary results and Young’s inequality, we obtain (similar but more detailed estimates are given in [9, pp. 1387 – 1388]):
\[|\Xi_1| \leq \sum_{F \in \mathcal{F}\cup\mathcal{F}_N} \left( C h_K \|e_u\|^2_{L^2(F)} + h_K^{-1} \|v \theta_u\|^2_{L^2(F)} \right)\]
\[\leq \|e_u\|^2_{L^2(\Omega)} + C \|v\|^2_{L^\infty(\Omega)} \|u\|^2_{H^{k+1}(\Omega)} h^{2k},\]
\[|\Xi_2| \leq \sum_{K \in h} h_K^2 \|e_u\|^2_{H^1(K)} + \sum_{K \in h} h_K^2 \|v \theta_u\|^2_{L^2(K)}\]
\[\leq \|e_u\|^2_{L^2(\Omega)} + C \|v\|^2_{L^\infty(\Omega)} h^{2k} \|u\|^2_{H^{k+1}(\Omega)},\]
\[|\Xi_3| \leq \frac{1}{2} \|\nabla \cdot v\|^2_{L^\infty(\Omega)} \|e_u\|^2_{L^2(\Omega)}\]
5.3.3 Numerical results

<table>
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<tr>
<th>i</th>
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<th>$|u_h - u|$</th>
<th>EOC</th>
<th>$|q_h - q|$</th>
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Table 5.5: Convergence results for $P^0 - P^0$ approximation.

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<th>EOC</th>
<th>$|q_h - q|$</th>
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Table 5.6: Convergence results for $P^1 - P^0$ and $P^1 - P^1$ approximations.

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<th>$|q_h - q|$</th>
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<td>2.07</td>
</tr>
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</table>

Table 5.7: Convergence results for $P^2 - P^1$ and $P^2 - P^2$ approximations.

In this section, numerical results illustrating the performance of the method are presented. Choosing $\Omega = [0, 1] \times [0, 1]$, we use the following parameters

\[
T = 1, \quad \Delta t = 10^{-5}, \quad \eta = 10, \quad D = 0.5, \quad \nu = 0.5 \begin{pmatrix} \exp(0.5(x + y)) \\ \exp(0.5(x - y)) \end{pmatrix},
\]

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5.4 A hybridizable LDG scheme for Darcy’s equation including jump conditions

with a source term \( f \), flux boundary conditions on the left and bottom edges, and Neumann boundary conditions on the right and top edges chosen such that \( u = \cos(x_1 + t) \cos(x_2 + t) \) is the analytical solution of (5.8). The discretization and the implementation are analogous to those presented in [139, 159, 10]. The \( L^2 \)-errors and the experimental orders of convergence (EOC) are given in Tables 5.5 – 5.7. Results presented in Tables 5.5 – 5.7 clearly demonstrate the sharpness of our estimates and support our claim that, similarly to the pure diffusion case, by relying on flux approximations of one order lower than the primary unknowns, one still has the same convergence rates and similar values of the discretization error.

5.4 A hybridizable LDG scheme for Darcy’s equation including jump conditions and using different approximation spaces

In the following, we investigate an LDG-H method — a particular type of HDG scheme [130] related to LDG discretizations — using numerical experiments and analyze its stability and convergence when applied to instationary equations with non-linear tensor-valued diffusion coefficients exemplified by Darcy flows. Of special interest are approximation spaces of different orders for different unknowns such as in the above sections and [130, 10]. Our formulation allows for non-linear diffusion tensors and enforces jumps in the primary unknown described by Henry’s law. The analysis relies in part on techniques employed for the LDG formulations above (cf. Section 5.2.4) and in [1, 8–10], and extends them to the LDG-H method.

The existing convergence order estimates for the LDG-H method show remarkable results under high regularity assumptions also with respect to time. For some configurations, optimal convergence in both the scalar and the flux variables was shown. With additional assumptions, super-convergence in the average of the scalar variable can be shown which gives rise to the application of post-processing techniques [161]. In the following, we will review the most important existing results and extend some of these to cases including jump conditions.

The first analysis for a HDG-type method was given by Cockburn et al. in [127] for a special LDG-H variant called the single face hybridizable method; its distinctive feature is the penalty coefficient \( \tau \) — which will turn out to be different from \( \eta \) utilized for LDG methods — chosen as a positive constant on one face of each simplex and zero everywhere else. A more general result for elliptic problems followed in [126] and relied on a special projection (exclusively for
simplex-meshes) tailored to fit the characteristics of HDG methods. These results were generalized to non-conforming simplicial meshes in [120] and squares, cubes, and prisms in [128]. An analysis for a Poisson equation involving additive jumps in the primary and the flux unknowns (as opposed to multiplicative jumps considered here) was presented in [135], and parabolic problems with non-linear diffusion tensors were considered in [148].

Despite the outstanding convergence properties of HDG methods, there seems to be one major drawback. All the aforementioned proofs only work with much extra technical effort compared to the well-known results for classical DG methods. Instead of the $L^2$-projection, more elaborate projections are used, most often only defined on simplicial meshes. Producing similar results with fewer restrictions regarding mesh and regularity assumptions in time and space would be desirable. Nonetheless, a proof for the problem of Darcy flow with internal jumps and a general non-linear diffusion tensor (5.1) is presented in the following sections.

### 5.4.1 Spatial discretization

For the purpose of hybridizing an LDG method and solve the problem described in Section 5.2.1, another ansatz space — the so-called skeleton space on the element faces (excluding those with the Dirichlet boundary conditions) — needs to be defined:

$$\mathbb{P}_k (\mathcal{F}_{\bar{D}}) := \left\{ \mu \in L^2 \left( \bigcup_{F \in \mathcal{F}_{\bar{D}}} F \right) : \mu|_F \in \mathbb{P}_k (F), \forall F \in \mathcal{F}_{\bar{D}} \right\}.$$

For $F \in \mathcal{F}_I$, an interior face shared by cells $\mathcal{K}^-$ and $\mathcal{K}^+$, and for $x \in F$, we define the one-sided values of a scalar quantity $w = w(x)$ by

$$w^- (x) := \lim_{\varepsilon \to 0^+} w(x - \varepsilon \nu_{\mathcal{K}^-}) \quad \text{and} \quad w^+ (x) := \lim_{\varepsilon \to 0^+} w(x - \varepsilon \nu_{\mathcal{K}^+})$$

and for $F \in \mathcal{F}_{\Gamma}$, a face on $\Gamma_{LG}$ shared by cells $\mathcal{K}^l \subset \Omega^1$ and $\mathcal{K}^g \subset \Omega^g$, and for $x \in F$, we define the one-sided values of a scalar quantity $w = w(x)$ by

$$w^l (x) := \lim_{\varepsilon \to 0^+} w(x - \varepsilon \nu_{\mathcal{K}^l}) \quad \text{and} \quad w^g (x) := \lim_{\varepsilon \to 0^+} w(x - \varepsilon \nu_{\mathcal{K}^g}).$$

Additionally, a new variable on the skeleton space $\mathbb{P}_k (\mathcal{F}_{\bar{D}})$ is introduced and denoted by $\lambda_h$.

In the following, a modification of the LDG-H method described in [161] is proposed — capable of dealing with jump conditions along a submanifold $\Gamma_{LG}$ (i.e.
Henry’s law) and using instationary Darcy flow as an example application. This is exactly the problem described in Section 5.2.1 which will be treated in the following.

To deal with Henry’s law, the numerical trace $\hat{u}_h$ is defined as

$$\hat{u}_h|_{\partial \mathcal{K}} := \begin{cases} u_D & \partial \mathcal{K} \cap \partial \Omega_D \\ \lambda_h & \partial \mathcal{K} \setminus (\partial \Omega_D \cup \Gamma_{LG}) \\ \lambda_h & (\partial \mathcal{K} \cap \Gamma_{LG}) \cap (\mathcal{K} \subset \Omega^s) \\ H_{LG} \lambda_h & (\partial \mathcal{K} \cap \Gamma_{LG}) \cap (\mathcal{K} \subset \Omega^l) \end{cases}$$

whereas the numerical flux $\hat{q}_h$ is chosen as

$$\hat{q}_h|_{\partial \mathcal{K}} := q_h + \tau (u_h - \hat{u}_h) \nu_{\mathcal{K}},$$

where $\tau \geq 0$ is a stabilization parameter (possibly depending on $h$). For more information on the stabilization parameter $\tau$, the reader is referred to [127, 129]. The (semi-discrete) LDG-H formulation of the model problem (5.1) reads:

**Problem 5.4.1 (Semi-discrete LDG-H problem for Henry’s law).** Find a tripe of functions $(u_h, q_h, \lambda_h) \in P_k (T_h) \times P_{k-1}^d (T_h) \times P_{k-1} (F \setminus F_D)$ such that (5.12) holds for all test functions $(\varphi_u, \varphi_q, \varphi_\lambda) \in P_k (T_h) \times P_{k-1}^d (T_h) \times P_{k-1} (F \setminus F_D)$, all $\mathcal{K} \in T_h$, and a.e. $t \in (0, T)$

\[
\begin{align*}
\int_{\mathcal{K}} \partial_t u_h \varphi_u \, dx - \int_{\mathcal{K}} q_h \cdot \nabla \varphi_u \, dx + \int_{\partial \mathcal{K} \setminus (\partial \Omega_D \cup \Gamma_{LG})} (q_h \cdot \nu_{\mathcal{K}} + \tau (u_h - \lambda_h)) \varphi_u \, d\sigma \\
+ \int_{\partial \mathcal{K} \cap \Gamma_{LG}} \left( q_h \cdot \nu_{\mathcal{K}} + \begin{cases} \tau (u_h - H_{LG} \lambda_h) & \text{if } \mathcal{K} \subset \Omega^l \\ \tau (u_h - \lambda_h) & \text{if } \mathcal{K} \subset \Omega^s \end{cases} \right) \varphi_u \, d\sigma \\
+ \int_{\partial \mathcal{K} \cap \Gamma_D} (q_h \cdot \nu + \tau (u_h - u_D)) \varphi_u \, d\sigma = \int_{\mathcal{K}} f \varphi_u \, dx,
\end{align*}
\]

\[
\begin{align*}
\int_{\mathcal{K}} D^{-1} (u_h) q_h \cdot \varphi_q \, dx - \int_{\mathcal{K}} u_h (\nabla \cdot \varphi_q) \, dx + \int_{\partial \mathcal{K} \setminus (\partial \Omega_D \cup \Gamma_{LG})} \lambda_h \varphi_q \cdot \nu_{\mathcal{K}} \, d\sigma \\
+ \int_{\partial \mathcal{K} \cap \Gamma_{LG}} \left( \begin{cases} H_{LG} \lambda_h & \text{if } \mathcal{K} \subset \Omega^l \\ \lambda_h & \text{if } \mathcal{K} \subset \Omega^s \end{cases} \right) \varphi_q \cdot \nu_{\mathcal{K}} \, d\sigma + \int_{\partial \mathcal{K} \cap \Gamma_D} u_D \varphi_q \cdot \nu \, d\sigma = 0,
\end{align*}
\]

\[
\begin{align*}
\sum_{F \in T} \int_F (\| q_h \| + \tau (u_h^+ + u_h^- - 2 \lambda_h)) \varphi_\lambda \, d\sigma + \sum_{F \in T} \int_F (q_h \cdot \nu + \tau (u_h - \lambda_h)) \varphi_\lambda \, d\sigma \\
+ \sum_{F \in T} \int_F (\| q_h \| + \tau (u_h^+ + u_h^- - (1 + H_{LG}) \lambda_h)) \varphi_\lambda \, d\sigma = \sum_{F \in T} g_N \varphi_\lambda \, d\sigma.
\end{align*}
\]
Here, $k$, $\hat{k}$, $\bar{k}$ denote orders of polynomial ansatz spaces for different unknowns.

**Remark 5.4.2.** (5.12c) is a globally coupled system that ensures the local mass conservation, whereas (5.12a), (5.12b) are element-local and can be solved element by element.

### 5.4.2 Stability estimate

The analysis heavily relies on techniques presented in Section 5.2.4 and in [1, 8–10], additional results used in the proofs are introduced in the corresponding sections. First, a new function $\tilde{H}^{LG}(x)$ that generalizes the Henry coefficient to the whole domain $\Omega$ is defined (note that argument $x$ is omitted later on):

$$
\tilde{H}^{LG}(x) := \begin{cases} 
1 & x \in \overline{\Omega} \setminus \Gamma_{LG}, \\
H_{LG}^{\Gamma} & x \in \Omega^s.
\end{cases}
$$

**Theorem 5.4.3 (Energy stability of the semi-discrete problem).** Assume that $(u_h, q_h)$ satisfy Problem 5.4.1. For every regular, geometrically conformal family of meshes $(T_h^T)_{h>0}$ and for all $\tau, h > 0$ in (5.12), there exists a function $C$ such that for a.e. $s \in (0, T)$

$$
\left\| \sqrt{\tilde{H}^{LG}} u_h(s, \cdot) \right\| \Omega^2 + \int_0^s \left\| \sqrt{\tilde{H}^{LG}} D^{-1}(u_h) q_h \right\|^2 \Omega \\
+ \sum_{F \in T \setminus T_D} \tau \tilde{H}^{LG} \left\| \lambda_h \right\|^2_F + \sum_{F \in T_D} \tau \tilde{H}^{LG} \left\| u_h \right\|^2_F \right\| d t \leq C(s).
$$

**Proof.** The proof uses ideas from the proof of Theorem 5.2.13 / [10, Theorem 4.9]. Special care must be taken of the boundary with the specified jump condition $\Gamma_{LG}$.

We test equations (5.12) with $\tilde{H}^{LG} u_h, \tilde{H}^{LG} q_h$, and $-\tilde{H}^{LG} \lambda_h$, integrate the second equation by parts, and sum the first two over all $K \in T_h$. This yields

$$
\int_{\Omega} (\partial_t u_h) \tilde{H}^{LG} u_h \, dx - \sum_{K \in T_h} \int_K \tilde{H}^{LG} q_h \cdot \nabla u_h \, dx \\
+ \sum_{F \in T_D} \int_F (q_h \cdot v + \tau (u_h - u_D)) \tilde{H}^{LG} u_h \, d\sigma
$$
Adding the above equations together and using algebraic simplifications gives

\[
\begin{align*}
&+ \sum_{F \in T_i} \int_{F} \left( \frac{\hat{H}^{\text{LG}}}{\hat{H}^{\text{LG}}} q_h u_h \right) + \tau \left( u_h^\pm - \lambda_h \right) \frac{\hat{H}^{\text{LG}}}{\hat{H}^{\text{LG}}} u_h^\pm + \tau \left( u_h^\pm - \lambda_h \right) \frac{\hat{H}^{\text{LG}}}{\hat{H}^{\text{LG}}} u_h^\pm \, d\sigma \\
&+ \sum_{F \in T_f} \int_{F} \left( \| q_h \hat{H}^{\text{LG}} u_h \| + \tau \left( u_h^l - \hat{H}^{\text{LG}} \lambda_h \right) u_h^l + \tau \left( u_h^g - \lambda_h \right) \hat{H}^{\text{LG}} u_h^g \right) \, d\sigma \\
&+ \sum_{F \in T_{N}} \int_{F} (q_h \cdot v + \tau (u_h - \lambda_h)) \hat{H}^{\text{LG}} u_h \, d\sigma = \int_{\Omega} f \hat{H}^{\text{LG}} u_h \, dx, \\
&\int_{\Omega} D^{-1} (u_h \hat{H}^{\text{LG}} q_h \cdot q_h) \, dx + \sum_{K \in T_h} \int_{K} \hat{H}^{\text{LG}} \nabla u_h \cdot q_h \, dx \\
&- \sum_{F \in (T_h \cup T_l)} \int_{F} \| u_h \hat{H}^{\text{LG}} q_h \| \, d\sigma - \sum_{F \in (T_h \cup T_N)} \int_{F} u_h \hat{H}^{\text{LG}} q_h \cdot v \, d\sigma \\
&+ \sum_{F \in T_i} \int_{F} \lambda_h \hat{H}^{\text{LG}} \| q_h \| \, d\sigma + \sum_{F \in T_N} \int_{F} \lambda_h \hat{H}^{\text{LG}} q_h \cdot v \, d\sigma \\
&+ \sum_{F \in T_D} \int_{F} u_D \hat{H}^{\text{LG}} q_h \cdot v \, d\sigma + \sum_{F \in T_t} \int_{F} \lambda_h \hat{H}^{\text{LG}} \| q_h \| \, d\sigma = 0, \\
&\sum_{F \in T_i} \int_{F} \left( \| q_h \| + \tau \left( u_h^\pm - \lambda_h + u_h^\pm - \lambda_h \right) \right) \left( -\hat{H}^{\text{LG}} \lambda_h \right) \, d\sigma \\
&+ \sum_{F \in T_f} \int_{F} \left( \| q_h \| + \tau \left( u_h^l - \hat{H}^{\text{LG}} \lambda_h + u_h^g - \lambda_h \right) \right) \left( -\hat{H}^{\text{LG}} \lambda_h \right) \, d\sigma \\
&+ \sum_{F \in T_N} \int_{F} (q_h \cdot v + \tau (u_h - \lambda_h)) \left( -\hat{H}^{\text{LG}} \lambda_h \right) \, d\sigma \\
&= \sum_{F \in T_N} \int_{F} g_N \left( -\hat{H}^{\text{LG}} \lambda_h \right) \, d\sigma.
\end{align*}
\]

Adding the above equations together and using algebraic simplifications gives

\[
\frac{1}{2} \partial_t \| \sqrt{\hat{H}^{\text{LG}}} u_h \|_{\Omega}^2 + \left\| \sqrt{\hat{H}^{\text{LG}}} D^{-1} (u_h) q_h \right\|_{\Omega}^2 + \sum_{F \in T_N} \tau \hat{H}^{\text{LG}} \left( \| u_h \|_{F}^2 + \| \lambda_h \|_{F}^2 \right) \\
+ \sum_{F \in T_i} \tau \hat{H}^{\text{LG}} \left( \| u_h \|_{F}^2 + \| u_h^\pm \|_{F}^2 + 2 \| \lambda_h \|_{F}^2 \right) + \sum_{F \in T_D} \tau \hat{H}^{\text{LG}} \| u_h \|_{F}^2 \\
+ \sum_{F \in T_f} \tau \left( \| u_h^l \|_{F}^2 + \hat{H}^{\text{LG}} \| u_h^g \|_{F}^2 + \hat{H}^{\text{LG}} \left( \hat{H}^{\text{LG}} + 1 \right) \| \lambda_h \|_{F}^2 \right)
\]

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\[ = \int_{\Omega} \tilde{H}^{LG} f u_h \, dx - \sum_{F \in \mathcal{N}} \tilde{H}^{LG} \int_{F} g_{N \lambda_h} \, ds + \sum_{F \in \mathcal{I}_1} \tau \tilde{H}^{LG} \int_{F} 2 \lambda_h (u_h^- + u_h^+) \, ds \]

\[ + \sum_{F \in \mathcal{I}_2} \tau H^{LLG} \int_{F} 2 \lambda_h (u_h^+ + u_h^0) \, ds + \sum_{F \in \mathcal{N}} \tilde{H}^{LG} \int_{F} 2 \lambda_h u_h \, ds \]

\[ + \sum_{F \in \mathcal{I}_4} \tau \tilde{H}^{LG} \int_{F} u_D u_h \, ds - \sum_{F \in \mathcal{I}_7} \tilde{H}^{LG} \int_{F} u_D q_h \cdot v \, ds. \]

Using Young’s, Cauchy–Schwarz’ inequalities, and Lemma 5.2.6, the \( \Xi_i \) terms can be estimated as follows:

\[ \left| \Xi_1 \right| \leq \frac{1}{2} \| \sqrt{\tilde{H}^{LG} f} \|_{\Omega}^2 + \frac{1}{2} \| \sqrt{\tilde{H}^{LG} u_h} \|_{\Omega}^2 \]

\[ \left| \Xi_2 \right| \leq \sum_{F \in \mathcal{N}} \tilde{H}^{LG} \left( \frac{1}{t} \| g_{N \lambda_h} \|_{\tilde{F}}^2 + \frac{\tau}{4} \| \lambda_h \|_{\tilde{F}}^2 \right) \]

\[ \left| \Xi_3 \right| \leq \sum_{F \in \mathcal{I}_1} \tau \tilde{H}^{LG} \left( \| \lambda_h \|_{\tilde{F}}^2 + \| u_h^+ \|_{\tilde{F}}^2 + \frac{1}{2} \| \lambda_h \|_{\tilde{F}}^2 + 2 \| u_h^+ \|_{\tilde{F}}^2 \right) \]

\[ \left| \Xi_4 \right| \leq \sum_{F \in \mathcal{I}_2} \tau \left( (H^{LLG})^2 \| \lambda_h \|_{\tilde{F}}^2 + \| u_h^+ \|_{\tilde{F}}^2 + H^{LLG} \left( \frac{1}{2} \| \lambda_h \|_{\tilde{F}}^2 + 2 \| u_h^+ \|_{\tilde{F}}^2 \right) \right) \]

\[ \left| \Xi_5 \right| \leq \sum_{F \in \mathcal{N}} \tilde{H}^{LG} \left( \frac{1}{4} \| \lambda_h \|_{\tilde{F}}^2 + 4 \| u_h \|_{\tilde{F}}^2 \right) \]

\[ \left| \Xi_6 \right| \leq \sum_{F \in \mathcal{I}_2} \tau \tilde{H}^{LG} \left( \frac{1}{2} \| u_D \|_{\tilde{F}}^2 + \frac{1}{2} \| u_h \|_{\tilde{F}}^2 \right) \]

\[ \left| \Xi_7 \right| \leq \sum_{F \in \mathcal{I}_7} \tilde{H}^{LG} \frac{d C_D C_{tr}}{2 h_f} \| u_D \|_{\tilde{F}}^2 + \frac{1}{2} \int_{\Omega} \tilde{H}^{LG} D^{-1} (u_h) q_h \cdot q_h \, dx \]

Substituting the above estimates gives

\[ \partial_t \| \sqrt{\tilde{H}^{LG} u_h} \|_{\tilde{D}}^2 + \left\| \sqrt{\tilde{H}^{LG} D^{-1} (u_h)} q_h \right\|_{\Omega}^2 + \sum_{F \in \mathcal{I} \setminus \mathcal{I}_D} \tau \tilde{H}^{LG} \| \lambda_h \|_{\tilde{F}}^2 + \sum_{F \in \mathcal{I}_D} \tau \tilde{H}^{LG} \| u_h \|_{\tilde{F}}^2 \]

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\[ \leq \| \sqrt{H}LG f \|_{\Omega}^2 + \| \sqrt{H}LG u_h \|_{\Omega}^2 + \sum_{F \in F_N} \frac{2 HLG}{\tau} \| gN \|_{F}^2 + \sum_{F \in F_I} 2 \tau HLG \| u_h^+ \|_{F}^2 \]

+ \sum_{F \in F_T} 2 \tau HLG \| u_h^- \|_{F}^2 + \sum_{F \in F_N} 6 \tau HLG \| u_h \|_{F}^2 + \sum_{F \in F_D} \left( \tau + \frac{\tau \max}{h_F} \right) HLG \| u_D \|_{F}^2.

The stability result follows from first using Lemma 5.2.6 and then applying Grönwall’s inequality. □

5.4.3 Convergence order estimates

In the following, \( \tilde{k} \) and \( \bar{k} \) are set to \( k \), and the mesh is assumed to be simplicial. The convergence analysis of the semi-discrete scheme given in Problem 5.4.1 relies on a special type of Projection \( (\Pi_v, \Pi_w) \) introduced in [126] and also used in [119]. It is defined on each simplex \( K \) as

\[
\int_K \Pi_v q \cdot v \, dx = \int_K q \cdot v \, dx \quad \forall v \in P_{k-1}(K), \\
\int_K \Pi_w u w \, dx = \int_K uw \, dx \quad \forall w \in P_{k-1}(K), \\
\int_F \left( \Pi_v q \cdot v + \tau \Pi_w u \right) \mu \, d\sigma = \int_F \left( q \cdot v + \tau u \right) \mu \, d\sigma \quad \forall F \subset \partial K, \, \forall \mu \in P_k(F).
\]

The approximation properties of this projection are given in the following

**Lemma 5.4.4** (Corollary of Theorem 2.1 from [126]). Let \( \tau |\partial K \) be non-negative, and let \( \tau_{\max} := \max \tau |\partial K > 0 \). Then for \( k \geq 0 \) and for given \( u \in H^{k+1}(K) \) and \( q \in H^{k+1}(K) \), system (5.13) is uniquely solvable for \( \Pi_v q \) and \( \Pi_w u \). Furthermore, there exists a constant \( C_{||} \) independent of \( K \) and \( \tau \) such that

\[
\| \Pi_v q - q \|_\mathcal{K} \leq C_{||} h^{k+1} \left( |q|_{H^{k+1}(K)} + \tau_{\max} |u|_{H^{k+1}(K)} \right),
\]

\[
\| \Pi_w u - u \|_\mathcal{K} \leq C_{||} h^{k+1} \left( |u|_{H^{k+1}(K)} + \tau_{\max} |q|_{H^{k+1}(K)} \right),
\]

where \( | \cdot |_{H^{k+1}(K)} \) denotes the standard Sobolev semi-norm on \( H^{k+1}(K) \). ♦

**Proof.** This corollary trivially follows from [126, Theorem 2.1] proved in the appendix of [126]. For \( k = 0 \), only the third equation of (5.13) makes sense and is sufficient to compute the projection. □
Remark 5.4.5. The fact that this analysis technique only works for simplex-shaped elements certainly constitutes a limitation of our methodology; however, our convergence results shown in Section 5.4.4 indicate that our scheme also converges with the same order for rectangular elements.

For the analytical solution \((u, q)\) and the discrete solution \((u_h, q_h)\) of our problem (5.1), we denote (in contrast, but similar to Section 5.2)

\[
\begin{align*}
\epsilon_u & := u_h - \Pi_w u, & \theta_u & := \Pi_w u - u, \\
\epsilon_q & := q_h - \Pi_v q, & \theta_q & := \Pi_v q - q, \\
\epsilon_\lambda^g & := \lambda_h - \Pi \lambda_h, & \theta_\lambda^g & := \Pi \lambda_h - \lambda_h, \\
\epsilon_\lambda^1 & := H^{\Gamma_\text{LG}} \lambda_h - \Pi u^1, & \theta_\lambda^1 & := \Pi u^1 - u^1,
\end{align*}
\]

Here, \(\Pi\) denotes an \(L^2\)-projection acting on a given \(\zeta \in L^2(\mathcal{F} \setminus \mathcal{T}_D)\). Note that the restriction of \(\Pi \zeta\) to \(F \in \mathcal{F} \setminus \mathcal{T}_D\) is in \(\mathbb{P}_k(F)\) and satisfies

\[
\Pi : F \to \mathbb{P}_k(F), \quad \int_F (\Pi \zeta - \zeta) \, \mu \, d\sigma = 0, \quad \forall \mu \in \mathbb{P}_k(F),
\]

similarly to \(\pi\) (acting on elements) from Section 5.2, and that \(H^{\Gamma_\text{LG}} e^g_\lambda = e^1_\lambda\) on \(\Gamma_\text{LG}\) since \(u^1 = H^{\Gamma_\text{LG}} u^g\) and \(\Pi\) is linear.

To deal with non-linear diffusion coefficients we state

Lemma 5.4.6. The following inequality holds true for \(u \in H^{k+1}(\Omega^a), u_h \in \mathbb{P}_k(\mathcal{T}_h),\)

\[
q \in L^\infty(\Omega^a)^d \cap H^{k+1}(\Omega^a)^d, \alpha = 1, g, \text{ and } e_q \text{ defined in (5.14)}:
\]

\[
\int_\Omega \left( D^{-1}(u_h) - D^{-1}(u) \right) q \cdot e_q \, dx \leq \varepsilon \|e_q\|_{L^2(\Omega)}^2 + \frac{L_D^2}{4\varepsilon} \|q\|_{L^\infty(\Omega)^d}^2 \left( \|e_u\|_{L^2(\Omega)}^2 + C^2_{H} \sum_{\mathcal{K} \in \mathcal{T}_h} \|u\|_{H^{k+1}(\mathcal{K})} + \frac{1}{\lambda_{\text{max}}} \|q\|_{H^{k+1}(\mathcal{K})^d}^2 \right)
\]

for some arbitrary \(\varepsilon > 0\).

Proof. Using Hölder’s, Young’s inequalities and properties of \(D^{-1}(\cdot)\) we obtain

\[
\int_\Omega \left( D^{-1}(u_h) - D^{-1}(u) \right) q \cdot e_q \, dx \leq \|q\|_{L^\infty(\Omega)^d} \|D^{-1}(u_h) - D^{-1}(u)\|_{\Omega} \|e_q\|_{\Omega}
\]

\[
\leq L_D \|u_h - u\|_{\Omega} \|q\|_{L^\infty(\Omega)^d} \|e_q\|_{\Omega} \leq \varepsilon \|e_q\|_{\Omega}^2 + \frac{L_D^2}{4\varepsilon} \|q\|_{L^\infty(\Omega)^d}^2 \left( \|e_u\|_{\Omega}^2 + \|\theta_u\|_{\Omega}^2 \right),
\]

and the result then follows by Lemma 5.4.4. \(\square\)
Remark 5.4.7. A result related to Lemma 5.4.6 is mentioned in Remark 5.2.12 / [10, Rem. 4.8] without proof. Here, the projection defined in Lemma 5.4.4 is used instead of the standard $L^2$-projection utilized in Section 5.2 / [10].

Next, we prove the main convergence result.

**Theorem 5.4.8 (Convergence order estimate for the LDG-H method).** Let $(u, q) \in H^1(0,T;H^{k+1}(\Omega^1 \cup \Omega^2)) \times H^1(0,T;H^{k+1}(\Omega^1 \cup \Omega^2)^d)$ be a solution to (5.1). Then for every regular, geometrically conformal family of simplicial meshes $T_h$ and a (for all $h > 0$) uniformly bounded parameter $\tau \geq \tau^*$ (for some $\tau^* > 0$), the solution of Problem 5.4.1 $(u_h, q_h)$ converges for almost every $s \in (0,T)$ with order $k + 1$ to the solution of Definition 5.2.2 $(u, q)$ in the following sense:

$$\|\sqrt{H}e_u(s, \cdot)\|^2_{L^2(\Omega)} + \int_0^s \left[ \|\sqrt{H}e_q\|^2_{L^2(\Omega)} + \sum_{F \in \mathcal{F}_N} \tau \|H e_u - e_{\lambda}\|^2_F 
+ \sum_{F \in \mathcal{F}_I} \tau \|H e_u\|^2_F + \sum_{F \in \mathcal{F}_D} \tau \left( \|e_u - e_{\lambda}\|^2_F + H e_u - e_{\lambda}\|^2_F \right) \right] dt \leq C h^{2k+2},$$

where $C$ is independent of $h$, and $\hat{k}, \tilde{k}$ from Problem 5.4.1 are chosen equal to $k$.

**Proof.** We use the consistency of the method, plug in the analytical and the discrete solution into (5.12), respectively, and subtract the resulting equations. Afterwards, we introduce $\pm \Pi_w u, \pm \Pi_v q$ terms into corresponding integrals in (5.12c), test the equations with $H e_u, H e_q, \text{and} -\tilde{H} e_{\lambda}$, respectively, integrate the second equation by parts, and sum over all $K \in T_h$. This yields

$$\int_\Omega \partial_t e_u H e_u \, dx - \sum_{K \in T_h} \int_K H e_q \cdot \nabla e_u \, dx + \sum_{F \in \mathcal{F}_D} \int_F (e_q \cdot v + \tau e_u) H e_u \, d\sigma$$

$$+ \sum_{F \in \mathcal{F}_I} \int_F \left( \|H e_q\| + \tau (e_u - e_{\lambda}) H e_u + \tau (e_u - e_{\lambda}) \tilde{H} e_u \right) \, d\sigma$$

$$+ \sum_{F \in \mathcal{F}_D} \int_F \left( \|H e_q\| + \tau (e_u - e_{\lambda}) H e_u + \tau (e_u - e_{\lambda}) \tilde{H} e_u \right) \, d\sigma$$

$$+ \sum_{F \in \mathcal{F}_N} \int_F (e_q \cdot v + \tau (e_u - e_{\lambda})) H e_u \, d\sigma = -\int_\Omega \partial_t \theta_u \tilde{H} e_u \, dx,$$

$$\int_\Omega D^{-1}(u_h) e_q \cdot \tilde{H} e_q \, dx + \sum_{K \in T_h} \int_K H \nabla e_u \cdot e_q \, dx - \sum_{F \in \mathcal{F}_D} \int_F H \|e_u e_q\| \, d\sigma.$$
Using Young’s and Cauchy-Schwarz’ inequalities as well as Lemma 5.4.6 we get

\[ \sum_{F \in \mathcal{F}_D} \int_F \varepsilon_u H^{LG} e_q \cdot \nu \, d\sigma - \sum_{F \in \mathcal{F}_T} \int_F \| e_u H^{LG} e_q \| \, d\sigma + \sum_{F \in \mathcal{F}_N} \int_F \tilde{H}^{LG} \| e_q \| \, d\sigma \]

\[ + \sum_{F \in \mathcal{F}_T} \int_F \left( e_{\lambda}^1 e_q^1 \cdot \nu_{\mathcal{K}}^1 + e_{\lambda}^2 H^{LG} e_{\lambda}^2 \cdot \nu_{\mathcal{K}}^2 \right) \, d\sigma + \sum_{F \in \mathcal{F}_N} \int_F e_{\lambda} \tilde{H}^{LG} e_q \cdot \nu \, d\sigma \]

\[ = - \int_{\Omega} \tilde{H}^{LG} \left( D^{-1}(u_h) \theta_q + (D^{-1}(u_h) - D^{-1}(u)) q \right) \cdot e_q \, dx, \]

\[ - \sum_{F \in \mathcal{F}_T} \int_F \left( \| e_q \| + \tau (e_u^+ + e_u^\lambda - 2e_{\lambda}) \right) \tilde{H}^{LG} e_{\lambda} \, d\sigma \]

\[ - \sum_{F \in \mathcal{F}_N} \int_F (e_q \cdot \nu + \tau (e_u - e_{\lambda})) \tilde{H}^{LG} e_{\lambda} \, d\sigma \]

\[ - \sum_{F \in \mathcal{F}_T} \int_F \left( \| e_q \| + \tau \left( e_u^1 - e_{\lambda}^1 + e_u^\lambda - e_{\lambda}^\lambda \right) \right) H^{LG} e_{\lambda} \, d\sigma = 0. \]

Most of the projection error terms vanish due to the orthogonality properties of the chosen projection specified in Lemma 5.4.4. Adding up the equations, simple algebraic manipulations, and Lemma 5.4.6 give us

\[ \frac{1}{2} \partial \| \sqrt{\tilde{H}^{LG} e_u} \|_{\Omega}^2 + \| \sqrt{\tilde{H}^{LG} D^{-1}(u_h) e_q} \|_{\Omega}^2 \]

\[ + \sum_{F \in \mathcal{F}_D} \tau \tilde{H}^{LG} \| e_u \|_F^2 + \sum_{F \in \mathcal{F}_N} \tau \tilde{H}^{LG} \| e_u - e_{\lambda} \|_F^2 \]

\[ + \sum_{F \in \mathcal{F}_T} \tau \tilde{H}^{LG} \left( \| e_u^+ - e_{\lambda}^\lambda \|_F^2 + \| e_u^\lambda - e_{\lambda}^\lambda \|_F^2 \right) + \sum_{F \in \mathcal{F}_T} \tau \left( \| e_u^1 - e_{\lambda}^1 \|_F^2 + H^{LG} \| e_u^\lambda - e_{\lambda}^\lambda \|_F^2 \right) \]

\[ = - \int_{\Omega} \tilde{H}^{LG} \partial \| \theta_u e_u \|_{\Omega} \]

\[ - \int_{\Omega} \tilde{H}^{LG} D^{-1}(u_h) \theta_q \cdot e_q \, dx \]

\[ - \int_{\Omega} \tilde{H}^{LG} \left( D^{-1}(u_h) - D^{-1}(u) \right) q \cdot e_q \, dx \]

Using Young’s and Cauchy-Schwarz’ inequalities as well as Lemma 5.4.6 we get

\[ |\Xi_1| \leq \frac{1}{2} \| \sqrt{\tilde{H}^{LG} e_u} \|_{\Omega}^2 + \frac{1}{2} C_h^2 \tilde{H}^{LG} h^{2k+2} \sum_{K \in \mathcal{T}_h} \left( \| \partial \| H^{k+1}(K) \| + \frac{1}{\tau_{\max}^K} \| \partial \| H^{k+1}(K) \| \right)^2 \]

\[ |\Xi_2| \leq \frac{1}{4} \| \sqrt{\tilde{H}^{LG} D^{-1}(u_h) e_q} \|_{\Omega}^2 \]

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\[ + C_D C_H^2 H^2 \sum_{K \in T_h} \left( |q|_{H^k+1}(\mathcal{K}) + \tau_{K}^{\max} |u|_{H^k+1}(\mathcal{K}) \right)^2 \]

\[ |\Xi_3| \leq \frac{1}{4C_D} \left( \sqrt{H^2 L} \, e_{\Omega}^2 \right)^2 + C_D L^2 \, H \left\| q \right\|_{L^\infty(\Omega)}^2 \bigg( \left\| e_u \right\|_{\Omega}^2 + C_D^2 H^2 \sum_{K \in T_h} \left( |u|_{H^k+1}(\mathcal{K}) + \frac{1}{\tau_{K}^{\max}} |q|_{H^k+1}(\mathcal{K}) \right)^2 \bigg) \]

The remainder of the proof boils down to some simple algebraic manipulations, omitting some non-negative left-hand-side terms, and using Grönwall's inequality.

\[ \square \]

**Remark 5.4.9.** The fact that the above estimates contain \( \tau \) in both numerator and denominator indicates that choosing \( \tau \) as a global constant is optimal in contrast to \( \tau = 1/h \), or \( \tau = h \), or any other \( h \)-dependent choice.

### 5.4.4 Numerical results

**Convergence study.** First, we verify the convergence estimates by using a smooth test problem with known solution. Our smooth test problem is

\[ T = 1, \quad \Delta t = 10^{-4}, \]
\[ \Omega^1 = (0, 10) \times (0, 5), \quad \Omega^8 = (0, 10) \times (5, 10), \]
\[ H^L = 10, \quad \tau \in \{ 1, 1/h \}, \]
\[ D = \begin{cases} 0.1 & \text{if } x_2 < 5, \\ 1 & \text{otherwise}, \end{cases} \]
\[ u = \begin{cases} 10 \cos (x_1 + t) \cos (x_2 + t) & \text{if } x_2 < 5, \\ \cos (x_1 + t) \cos (x_2 + t) & \text{otherwise}. \end{cases} \]

On a square of side length ten, the upper and lower boundaries are Neumann boundaries, while the left- and right-hand side boundaries are of Dirichlet type. The right-hand side, initial, and boundary conditions are chosen appropriately. The spatial domain is discretized by \( 2^i \times 2^i \) squares (where \( i \) denotes the number of refinement steps). The discretization in time is performed using an implicit Euler scheme with constant time step size \( \Delta t \). As the skeleton space grows with each mesh refinement, the error on the skeleton space is scaled with respect to the measure of the skeleton space. The implementation is carried out in the C++ based finite element toolbox M++ [43].
Choosing the penalty parameter \( \tau = 1 \) and using equal order approximations for all unknowns, the LDG-H-discretization shows an optimal order of convergence of \( k + 1 \) in both variables for ansatz spaces of order \( k \) (see Table 5.8 and Tables 5.9 – 5.10 uppermost block). Notably this means an improved order of convergence in the flux variable compared to the LDG-discretization of the same order. For \( \tau = 1/h \) the order of convergence in the flux variable decreases by one. This is consistent with analytical results and also with numerical studies for elliptic problems given in [129].

\[
\begin{array}{cccccc}
\text{Table 5.8: Errors and estimated orders of convergence (EOC) for constant approximations.} \\

\hline
i & \mathbb{P}_0 & \mathbb{P}_0 \times \mathbb{P}_d & \mathbb{P}_0 \times \mathbb{P}_1 & \mathbb{P}_1 \times \mathbb{P}_0 & \mathbb{P}_1 \times \mathbb{P}_1 \\
\hline
& \|u_h - u\| & \|q_h - q\| & \|\lambda_h - \lambda\| & \|u_h - u\| & \|q_h - q\| & \|\lambda_h - \lambda\| \\
1 & 2.21E+1 & 5.08E+0 & 2.68E+0 & 2.05E+1 & 4.91E+0 & 2.37E+0 \\
2 & 3.03E+1 & 6.22E+0 & 3.20E+0 & 3.00E+1 & 6.08E+0 & 3.13E+0 \\
3 & 3.74E-1 & 1.67E-1 & 1.70E-1 & 2.12E-1 & 2.78E-1 & 3.18E-2 \\
4 & 7.19E-1 & 4.85E-2 & 4.10E-3 & 1.96E-1 & 7.59E-3 & 2.06E-1 \\
5 & 1.53E+0 & 1.37E+0 & 2.12E+0 & 3.60E+0 & 2.05E+0 & 5.48E+0 \\
6 & 3.53E+0 & 3.13E+0 & 5.48E+0 & 5.48E+0 & 3.13E+0 & 5.48E+0 \\
\hline
\end{array}
\]

\[
\begin{array}{cccccc}
\text{Table 5.9: Errors and estimated orders of convergence (EOC) for linear approximations.} \\

\hline
i & \mathbb{P}_1 & \mathbb{P}_0 \times \mathbb{P}_d & \mathbb{P}_0 \times \mathbb{P}_1 & \mathbb{P}_1 \times \mathbb{P}_0 & \mathbb{P}_1 \times \mathbb{P}_1 \\
\hline
& \|u_h - u\| & \|q_h - q\| & \|\lambda_h - \lambda\| & \|u_h - u\| & \|q_h - q\| & \|\lambda_h - \lambda\| \\
1 & 2.21E+1 & 5.33E+0 & 2.81E+0 & 2.06E+1 & 5.17E+0 & 2.65E+0 \\
2 & 6.62E+0 & 3.49E+0 & 2.08E+0 & 6.32E+0 & 3.50E+0 & 2.03E+0 \\
3 & 1.74E+0 & 1.46E+0 & 8.40E-1 & 1.21E+0 & 1.81E+0 & 2.14E+0 \\
4 & 5.78E-1 & 9.41E-1 & 4.01E-1 & 5.78E-1 & 9.41E-1 & 2.14E-1 \\
5 & 2.57E-1 & 4.76E-1 & 2.32E-2 & 1.20E-1 & 9.32E-1 & 2.04E-1 \\
6 & 1.28E+0 & 9.74E-1 & 1.95E-1 & 6.45E+0 & 1.34E+0 & 6.61E-1 \\
\hline
\end{array}
\]
5.4 A hybridizable LDG scheme for Darcy’s equation including jump conditions

analytically that if the order was reduced for the flux variable by one to \( k - 1 \)
while the order for the scalar variable was still \( k \), both variables would converge
at least with order \( k \). In numerical experiments presented in Section 5.2 and [10],
the order of convergence for the scalar variable appeared to be higher than the
analytical result indicates, whereas the estimate for the flux variable was sharp.
Next, we investigate similar scenarios for our LDG-H scheme with penalty
parameter \( \tau = 1 \) and \( \tau = 1/h \), respectively. Since there is yet another ansatz space
to approximate the solution on element boundaries, there arises one additional
possibility to vary the order of approximation. For \( \tau = 1 \), the experimental order
of convergence for all variables decreases as soon as we reduce the order of one of
the approximation spaces. In the case of \( \tau = 1/h \) though, the order of convergence
decreases, when we reduce the order of approximation for the primary \( u_h \) or the hybrid variable \( \lambda_h \), and no convergence is detected if the order of
one of the corresponding spaces is 0. However, when we reduce the order
of the approximation space for the flux variable by one, the same effect as for
the LDG method occurs: The experimental order of convergence turns out to
be the same as for equal order approximations in all variables (Tabs. 5.9 – 5.10
third block). This indicates the possibility to reduce the number of the degrees
of freedom for the flux unknowns, and by doing this reduce the computational
effort necessary for an approximation of given accuracy.

<table>
<thead>
<tr>
<th>( h )</th>
<th>( \tau = 1 )</th>
<th>( \tau = 1/h )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( | u_h - u | )</td>
<td>( | q_h - q | )</td>
<td>( | u_h - u | )</td>
</tr>
<tr>
<td>1</td>
<td>2.81E+1</td>
<td>6.58E+0</td>
</tr>
<tr>
<td>2</td>
<td>8.50E+0</td>
<td>1.72</td>
</tr>
<tr>
<td>3</td>
<td>1.17E+0</td>
<td>2.85</td>
</tr>
<tr>
<td>4</td>
<td>1.41E-1</td>
<td>3.05</td>
</tr>
<tr>
<td>5</td>
<td>1.78E-2</td>
<td>2.98</td>
</tr>
</tbody>
</table>

Table 5.10: Errors and estimated orders of convergence (EOC) for quadratic approximations.
Nested rectangle problem. To demonstrate the robustness of our method we have a look at the results for a more involved non-smooth test problem given by

\[ T = 1, \quad \Delta t = 10^{-4}, \]
\[ \Omega^1 = (0, 10) \times (0, 5), \quad \Omega^8 = (0, 10) \times (5, 10), \]
\[ H_{LG}^1 = 0.5, \quad \tau = 1/h, \]
\[ D = \begin{cases} 0.1 & \text{if } x_2 < 5, \\ 4 & \text{otherwise,} \end{cases} \]
\[ u_0 = \begin{cases} 5 & \text{if } (2.5 \leq y \leq 5.0) \land (2.5 \leq x \leq 7.5) \\ \lor (3.75 \leq y \leq 5.0) \land (0.0 \leq x \leq 10.0), \\ 10 & \text{if } (5.0 \leq y \leq 7.5) \land (2.5 \leq x \leq 7.5) \\ \lor (5.0 \leq y \leq 6.25) \land (0.0 \leq x \leq 10.0), \\ 0 & \text{otherwise.} \end{cases} \]

On a square of side length ten, all boundaries are of Neumann type. The right-hand-side function and boundary conditions are homogeneous.

The initial condition for the nested rectangle problem is plotted in Figure 5.2 (top left), the solutions at time \( T = 1 \) for piecewise linear and piecewise quadratic (equal order) approximation are shown in Figure 5.2 (middle left) and Figure 5.2 (bottom left), respectively, and the difference plot between these two is displayed in Figure 5.2 (top right). In order to illustrate the effect of reducing by one the approximation order for the flux unknown \( q_h \), we also display the difference plots between equal and reduced (for \( q_h \)) order solutions for linear in Figure 5.2 (middle right) and quadratic in Figure 5.2 (bottom right) approximations. Especially for the piecewise quadratic approximation the difference between the solutions appears to be very small.

5.5 Conclusions and future prospects

We analyzed an LDG and an LDG-H method capable of dealing with a simple jump condition for Darcy flow. That is, we considered a simplification of Henry’s law, where the solubility constant \( H_{LG}^1 \) is a positive constant which does not depend on space, time, or the solution of the PDE. For LDG, our analytical and numerical results indicate that it is optimal to choose the polynomial degree for the primary unknown one order higher than that for the flux unknowns, since this induces the same order of convergence as choosing both ansatz spaces of the higher degree at lower computational costs. There is hope to extend this analysis to the case of a space- and time-dependent \( H_{LG}^1 \). The analysis of a non-linear \( H_{LG}^1 \) is still an open problem and needs to be considered in the future.
Figure 5.2: Solution for the nested rectangle problem (left panel): initial condition (top), final states at $T = 1$ for $P_1 \times P_2 \times P_1$ (middle) and $P_2 \times P_2 \times P_1$ (bottom). Difference plots (right panel): $u_h|P_2 \times P_2 \times P_2 - u_h|P_1 \times P_1 \times P_1$ (top), $u_h|P_2 \times P_2 \times P_2 - u_h|P_1 \times P_1 \times P_1$ (middle), $u_h|P_2 \times P_2 \times P_2 - u_h|P_2 \times P_2 \times P_2$ (bottom).

As a by-product of our analysis, we figured out that the choice of the auxiliary variable $q = -D(u) \nabla u$ for our problem has better properties than the also commonly used $q = -\sqrt{D(u)} \nabla u$ and $q = -\nabla u$, cf. for example [9]. This can,
Chapter 5  Analysis of the discontinuous Galerkin method for Darcy’s equation

at least for jumping tensors illustratively, be explained by the fact that choosing the “correct” $q$ ensures that there occur no boundary integrals containing $D(u)$. Thus, the harder to control boundary integrals vanish by the construction of the method itself.

For the LDG-H method, our analysis had to be restricted to simplex meshes. Nevertheless, optimal convergence estimates were proved, and numerical studies demonstrated the same convergence on rectangular meshes. Our numerical studies of varying order approximations indicate the same behavior as in the case of LDG discretizations, namely the possibility of reducing the approximation order for flux unknowns by one without any loss of convergence or accuracy if the penalty parameter $\tau$ is chosen from $O(h^{-1})$. Regardless, there seems to be no need for further investigations of this behavior, since the optimal choice for $\tau$ is from $O(1)$. This is underlined by the thesis’ analytical and numerical results and can also be deduced from the literature. However, extending the performed analysis to more general element shapes appears to be very desirable — though challenging — since it generalizes the LDG-H method in a way such that it can be used for discontinuous diffusion tensors as well as for jump conditions.

Beyond that, the consideration of DG methods from the IP family imposes the possibility to further reduce computational costs, flux limiting techniques could force the numerical solutions to be more physical and post-processing techniques could force it to be more accurate. A combination of such techniques, for sure, is worth analyzing.
Chapter 6
Conclusions and future prospects

This monograph presented a process-based, comprehensive model for structure formation in soils. This model includes different phases on several spatial scales, i.e.,

- a micro-scale, which itself consists of two scales, namely
  - the scale where a cellular automaton describes the “movement of particles” (evolution of biomass, solid, gas, fluid) and
  - the scale where a model based on partial differential equations (PDEs) describes “movement of particles” (diffusing chemical species, etc.)

influencing one another, and
- a macro-scale, which is affected by the upscaled quantities of the micro-scale.

Moreover, this model includes at least four temporal scales, i.e.,

- the scale of fast (that is equilibrium) chemical reactions,
- the scale of kinetic chemical reactions and of transport of chemical species on the micro-scale,
- the scale of the motion described by the cellular automaton method,
- the scale on which the processes resolved by the macroscopic simulation take place.

Moreover, physical relations can be expressed by interactions of the different spatial and temporal scales. The set up model includes many coupled effects on these scales and the PDE-based parts are discretized using the local discontinuous Galerkin (LDG) method on the micro-scale. From a mathematical point of view, there are challenges, since analytical solutions of PDEs in general cannot exist on discretely moving domains. However, from a process-based point of view, this is not a serious issue if the numerical approximation of the PDE is interpreted as approximation of the physical process itself. Exemplary in this
sense is the interpretation of the LDG scheme applied to the diffusion equation as a tool describing the effects of diffusion in the cellular domain: Within one cell, the gradient of the concentration of the chemical species is reduced, and, between cells, transfer of a chemical species by diffusion from cells with high concentrations to cells with low concentrations takes place. This approach utilizes the LDG method as a “good” physical approximation of the processes — not so much of the equations — that are being described.

In addition to this, this thesis indicates that parameters that are derived from a discretely moving micro-domain can be used for upscaled models and illustrates old and new approaches to predict diffusion in such upscaled models — provided that there is no gas phase. This, of course, is a restriction one should try to eliminate in the future. Beyond this, upscaling of other quantities (permeabilities, combined domains of Stokes and Darcy flow, etc.) would be desirable. Upscaling quantities for combined domains of Stokes and Darcy flow using LDG schemes is dealt with by Simon Zech, a student at the Chair of Applied Mathematics I, whose Master’s Thesis is co-supervised by Andreas Rupp. Furthermore, a bi-directional coupling of the macro- and the micro-model would be worth analyzing.

In excess of what has already been mentioned, the whole model has been implemented but not yet numerically analyzed in three spatial dimensions. Taking a closer look at the behavior of the three-dimensional model seems to be as interesting as investigating the effects of somewhat weighted parts of the model on different measurements (cf. Section 2.2.4). This task is addressed in a upcoming article by Andreas Rupp, Nadja Ray, Alexander Prechtel (FAU Erlangen), and Thomas Ritschel, Tom Guhra, Kai Uwe Totsche (University of Jena).

To the best knowledge of Andreas Rupp, there exists no LDG analysis of the Nernst–Planck equations as presented in Chapter 2 and no analysis of the interior penalty family applied to problems with jump conditions (cf. Chapter 5). Such analysis would be valuable, since these methods could further decrease the computational costs of running our model. Beyond this, the application of HDG methods to our model could help by both reducing computational costs and by increasing the accuracy of the scheme (at the cost of high implementation demands), possibly including non-linear post-processing techniques. A first step in this direction has been done in this thesis. Additionally, flux limiting techniques could help to ensure that the solution satisfies physical constraints, as non-negativity.

The whole model developed in this thesis should also be made more physical by introducing more realistic chemistry and rate functions. This is planned to be actualized by groups from Stuttgart (using similar approaches to model coal seams) and Erlangen (using the precise model to describe the rhizosphere).
Publications with coauthor Andreas Rupp


Publications referenced in Chapter 2


Publications referenced in Chapter 3


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