Development and Evaluation of Iterative Solution Strategies for Coupled Stokes-Darcy Problems

Ackermann, S.

Supervisor: Christoph Grüninger
Abstract

Simulations for many environmental and industrial problems model interactions between a free flow and a flow in a porous medium. They require a coupling method which exchanges the values between the two subproblems accordingly. Using a monolithic coupling method involves large systems which have to be solved with a global solver, even if the numerical behavior of the subproblems differs significantly. In an iterative coupling method, different solvers can be applied to exploit the weakly coupled structure of the problem. Within this work, an iterative coupling method is implemented into the existing framework DUNE-MultiDomain by using a domain decomposition technique and solving the subproblems successively. In the current implementation of the monolithic coupling method, an expensive direct solver has to be used. In the iterative approach, a direct solver is applied only to the Stokes subproblem, while a linear iterative solver is available for the Darcy subproblem. The iterative coupling method converges towards the exact solution for stationary and transient test cases. The monolithic method is faster for the tested problems, but might be overtaken by the iterative method for larger systems. A modification corresponding to the ASPIN method does not improve the accuracy of the iterative coupling method. Further investigations are required to implement faster subproblem solvers which are necessary to reduce the computing time of the iterative coupling method.
# Contents

1 Introduction ................................................. 1

2 Model and coupling concept .............................. 3
   2.1 Mathematical model ................................. 3
   2.2 Domain decomposition methods ....................... 6
   2.3 Iterative coupling for the Stokes/Darcy problem .... 7
   2.4 Additive Schwarz Preconditioned Inexact Newton .... 10

3 Implementation ........................................... 12
   3.1 Software .............................................. 12
   3.2 Discrete Stokes/Darcy problem ....................... 13
   3.3 MAC scheme ............................................ 14
   3.4 Iterative coupling method ............................. 16
   3.5 ASPIN method .......................................... 17

4 Numerical results ......................................... 20
   4.1 Poisson/Poisson problem .............................. 20
   4.2 Stationary Stokes/Darcy problem ....................... 24
   4.3 Transient Stokes/Darcy problem ....................... 29
   4.4 ASPIN method .......................................... 31

5 Summary and conclusion ................................ 34
1 Introduction

Many industrial and environmental problems are influenced by the interactions of a free flow domain and an adjacent porous medium. Examples for environmental problems are the effects of river contamination on the groundwater and the dehydration of soils due to evaporation caused by winds. Exemplary technical applications are the drying of products, such as food, and filtration processes. Understanding, analyzing and predicting these processes is a major issue. In most cases, the necessary experiments tend to be time-consuming, expensive and inflexible. Therefore, modeling processes with partial differential equations became an important tool in various research fields. While free flow is usually modeled with the Stokes equations, the porous medium is governed by Darcy’s law. The Stokes/Darcy model needs a coupling method for the exchange of values between the two subdomains according to the problem’s physical background. This coupling method is still subject of research since its accuracy and influence on the computing time are important factors for the whole simulation.

A monolithic coupling method has been applied to the Stokes/Darcy problem at the Department of Hydromechanics and Modelling of Hydrosystems in previous implementations, e.g. [3] and [20]. The large global system of equations arising due to the discretization is solved in one step with a direct solver. Within this thesis, an approach which exploits the weakly coupled structure of the Stokes/Darcy problem is implemented and examined: the iterative coupling method, where both subdomains are solved successively.

Monolithic coupling does not enable the use of different linear solvers for the Stokes and Darcy subproblems. Therefore, an expensive direct solver is applied with a Newton’s method to the whole model domain, even if one of the subproblems is linear. This requires high computational effort and restricts the problem to small domains or low resolutions. The iterative approach seems to be promising for realistic scenarios, because the subdomain solvers can be chosen depending on the subproblem’s numerical behavior. Solving one subproblem with a linear solver and therefore reducing the size of the nonlinear system should speed up the computations. Additionally, this approach could be the base for further improvements such as applying different spatial grids or different time steps in each subdomain.
The mathematical background of domain decomposition methods for homogeneous as well as heterogeneous problems is presented in [24]. An iterative coupling method for a Poisson/Poisson problem with a cell-centered finite volume discretization is implemented in [1]. A finite element discretization for the iterative coupling of surface water with groundwater is analyzed in [13] and [18]. These works present proofs for the existence of weak solutions and the well-posedness of the global model. Algorithms and numerical results for both steady and time-dependent problems are given in [12].

The aim of this thesis is to realize and to evaluate the iterative coupling for Stokes/Darcy problems within the Distributed and Unified Numerics Environment (DUNE, [4]), using existing code for the solution of the Stokes and Darcy subproblems. Insights into the potential and complexity of iterative coupling in practice are desired.

The first step towards this aim is to implement the iterative Stokes/Darcy coupling for stationary problems. Its convergence behavior is analyzed and the computing times are compared to the monolithic method for several test cases. Then, the coupling method is extended to transient problems with transient boundary conditions. Furthermore, a possible improvement for high Reynolds numbers in Navier-Stokes/Darcy problems is implemented: A nonlinear domain decomposition preconditioner instead of the above described linear domain decomposition method is applied with the aim to extend the algorithm’s convergence to a broader range of application scenarios. Simple tests are used to determine the accuracy of this modified coupling method.

The following chapter explains the mathematical model, the iterative coupling concept and a method to tackle realistic parameter values. Chapter 3 treats aspects and difficulties concerning the implementation. In chapter 4 results of the numerical experiments for the Poisson/Poisson as well as the Stokes/Darcy problem are presented and interpreted. The last chapter is a summary and conclusion of this thesis.

I would like to thank the International Research Training Group NUPUS for the scholarship I received during the preparation of this work. It allowed me to focus on my thesis and to gain insights into related research topics in talks and presentations.
2 Model and coupling concept

This chapter contains the fundamental ideas and concepts of the coupled Stokes/Darcy problem. The mathematical equations in section 2.1 describe the behavior of fluids in free flow and porous media. Combining these equations with the domain decomposition approach in section 2.2 delivers an iterative coupling method for the Stokes/Darcy problem, see section 2.3. Section 2.4 presents a possible improvement to obtain a more robust algorithm.

2.1 Mathematical model

Two systems of partial differential equations describe the Stokes/Darcy problem mathematically. Additional conditions for the boundaries and the coupling interface close the model. An isothermal one-phase model is used in the following description, similar to [13]. A multi-phase formulation can be found in [20].

The model domain Ω is decomposed into two nonoverlapping subdomains Ω_{ff} and Ω_{pm}. The interface Γ separates the subdomains such that $\bar{\Omega} = \bar{\Omega}_{ff} \cup \bar{\Omega}_{pm}$, $\Omega_{ff} \cap \Omega_{pm} = \emptyset$ and $\bar{\Omega}_{ff} \cap \bar{\Omega}_{pm} = \Gamma$.

The Navier-Stokes equations are commonly used to model the flow of viscous fluids, such as water and air. Two balance equations for momentum and mass build a system of nonlinear partial differential equations for the free-flow subdomain $\Omega_{ff}$:

$$\frac{\partial}{\partial t}(\varrho v_{ff}) + \nabla \cdot (\varrho v_{ff}v_{ff}^T) - \nabla \cdot (\varrho \nu \nabla v_{ff}) + \nabla p_{ff} = q_{mom} \quad \text{in } \Omega_{ff}, \quad (2.1)$$

$$\frac{\partial}{\partial t} \varrho + \nabla \cdot (\varrho v_{ff}) = q_{mass,ff} \quad \text{in } \Omega_{ff}, \quad (2.2)$$

with the free-flow velocity $v_{ff}$ and the pressure $p_{ff}$ as primary unknowns. The kinematic viscosity $\nu > 0$ and the density $\varrho$ are properties of the fluid. The first two terms in equation (2.1) represent the inertial forces. The nonlinear advective term $\nabla \cdot (\varrho v_{ff}v_{ff}^T)$ generally makes these equations difficult to solve. Sink or source terms are given by
\( q_{\text{mom}} \) and \( q_{\text{mass,ff}} \). The two remaining terms correspond to the viscous and pressure forces.

If the advective inertial forces are small compared to the viscous forces, the second term in equation (2.1) can be dropped. This assumption is valid for slow flows with small Reynolds numbers \( (Re_{\text{ff}} < 1) \) and results in the linear Stokes equation

\[
\frac{\partial}{\partial t} (\rho \mathbf{v}_{\text{ff}}) - \nabla \cdot (\rho \mathbf{v}_{\text{ff}} \mathbf{v}_{\text{ff}}^T) + \nabla p_{\text{ff}} = q_{\text{mom}} \quad \text{in } \Omega_{\text{ff}}. \tag{2.3}
\]

The momentum balance for the porous medium subdomain \( \Omega_{\text{pm}} \) is described by Darcy’s law, which can be derived from the Navier-Stokes equations by averaging over a representative elementary volume. Assuming very slow flow velocities \( (Re_{\text{pm}} < 1) \) and neglecting gravitational forces leads to the fluid velocity being given as

\[
\mathbf{v}_{\text{pm}} = -\frac{K}{\mu} \nabla p_{\text{pm}} \quad \text{in } \Omega_{\text{pm}}, \tag{2.4}
\]

with the dynamic viscosity \( \mu \) and the intrinsic permeability tensor \( K \), which depends on properties of both the fluid and the porous medium. The mass balance equation for the flow through a porous medium reads

\[
\Phi \frac{\partial}{\partial t} \rho - \nabla \cdot (\rho \mathbf{v}_{\text{pm}}) = q_{\text{mass,pm}} \quad \text{in } \Omega_{\text{pm}}. \tag{2.5}
\]

The porosity \( \Phi \) arises in the averaging process over the porous medium and describes the ratio of void space volume and total volume.

Substituting \( \mathbf{v}_{\text{pm}} \) in equation (2.5) with the right-hand side of equation (2.4) and using the relation \( \nu = \rho / \rho \) for the kinematic viscosity leads to

\[
\Phi \frac{\partial}{\partial t} \rho + \nabla \cdot \left( -\frac{K}{\nu} \nabla p_{\text{pm}} \right) = q_{\text{mass,pm}} \quad \text{in } \Omega_{\text{pm}}, \tag{2.6}
\]

with the pressure \( p_{\text{pm}} \) being the only primary variable in \( \Omega_{\text{pm}} \). Therefore, the flow velocity in the porous medium \( \mathbf{v}_{\text{pm}} \) is eliminated.

Combining the balance equations for the two subproblems results in the following set of equations for the Navier-Stokes/Darcy problem:

\[
\frac{\partial}{\partial t} (\rho \mathbf{v}_{\text{ff}}) + \nabla \cdot (\rho \mathbf{v}_{\text{ff}} \mathbf{v}_{\text{ff}}^T) - \nabla \cdot (\rho \nu \nabla \mathbf{v}_{\text{ff}}) + \nabla p_{\text{ff}} = q_{\text{mom}} \quad \text{in } \Omega_{\text{ff}}, \tag{2.7}
\]

\[
\nabla \cdot (\rho \mathbf{v}_{\text{ff}}) = q_{\text{mass,ff}} \quad \text{in } \Omega_{\text{ff}}, \tag{2.8}
\]

\[
\Phi \frac{\partial}{\partial t} \rho + \nabla \cdot \left( -\frac{K}{\nu} \nabla p_{\text{pm}} \right) = q_{\text{mass,pm}} \quad \text{in } \Omega_{\text{pm}}. \tag{2.9}
\]
Replacing equation (2.7) with (2.3) yields the Stokes/Darcy problem.

The boundary conditions at the external boundary $\partial \Omega$ do not influence the coupling method, but are needed for a unique solution of the Stokes/Darcy problem. The boundary condition types and the respective boundary values depend on the actual problem and are given in chapter 4. The same applies to initial conditions which become necessary for transient problems.

**Coupling**

Three interface conditions at the interface $\Gamma$ supplement the model. They require the two subdomains to be in thermodynamic equilibrium, which is reached by mechanical, thermal and chemical equilibrium. Thermal and chemical equilibrium are not taken into account within this work, because an isothermal model with only one component is used. Multi-component and nonisothermal interface conditions are given in [3].

Due to the permeability of the interface, the normal velocities have to be continuous across $\Gamma$. This can be guaranteed by fulfilling the first condition for continuity of mass

\[
\mathbf{v}_\text{ff} \cdot \mathbf{n} = \left( \frac{K}{\mu} \nabla p_{\text{pm}} \right) \cdot \mathbf{n} \quad \text{on } \Gamma, \quad (2.10)
\]

where $\mathbf{n}$ is the unit outer normal vector of $\Omega_{\text{ff}}$.

Two coupling conditions are required for the continuity of momentum across the interface. The normal part is given by the continuity of stresses, which relates the pressures in the two subdomains across $\Gamma$. Therefore, the following equation has to be fulfilled:

\[
p_{\text{pm}} = p_{\text{ff}} + \mathbf{n} \cdot (\varrho \mathbf{v}_\text{ff}^T - \varrho \nu \nabla \mathbf{v}_\text{ff}) \mathbf{n} \quad \text{on } \Gamma, \quad (2.11)
\]

This condition is adapted to Stokes flow by neglecting the nonlinear advective term, yielding

\[
p_{\text{pm}} = p_{\text{ff}} + \mathbf{n} \cdot (-\varrho \nu \nabla \mathbf{v}_\text{ff}) \mathbf{n} \quad \text{on } \Gamma. \quad (2.12)
\]

A condition for the tangential velocity component in the free-flow domain $\Omega_{\text{ff}}$ is given by the Beavers-Joseph-Saffman condition

\[
(\nabla \mathbf{v}_\text{ff}) \cdot \mathbf{t}_j = -\frac{\alpha_{BJ}}{\sqrt{K_{j,j}}} \mathbf{v}_\text{ff} \cdot \mathbf{t}_j \quad \text{on } \Gamma, \quad (2.13)
\]

with the tangential vectors at the interface $\mathbf{t}_j$. Since this condition does not depend on $p_{\text{pm}}$, it is actually a boundary condition for the free-flow domain $\Omega_{\text{ff}}$. 


2.2 Domain decomposition methods

The basic idea of domain decomposition is to partition a given computational domain $\Omega$ into $M$ subdomains $\Omega_i$, $i = 1, ..., M$. This decomposition can be applied to homogeneous as well as heterogeneous problems. In both cases, the subproblems of reduced size have to be coupled with each other by exchanging the values of the primary variables at the subdomain interfaces. Splitting the model domain of a homogeneous problem into smaller subdomains leads to $M$ reduced systems, which are all governed by the same equations. Heterogeneous problems, where the model domains are governed by different systems of partial differential equations, can be decomposed into subdomains according to these subsystems. Special coupling methods which fit to the respective primary variables of each subdomain become necessary.

By decomposing the global problem into local subproblems, smaller systems of equations have to be solved than for the global problem. Furthermore, different numerical schemes can be used within the subdomains to adapt to the respective behavior of the solution. Another advantage of domain decomposition is the possibility for parallel algorithms, solving all subdomains simultaneously on different processors.

In the following, the basic idea of domain decomposition is explained for the homogeneous Poisson problem

$$- \Delta u = f \text{ in } \Omega, \quad u = 0 \text{ on } \partial \Omega. \quad (2.14)$$

If $\Omega$ is divided into two nonoverlapping domains $\Omega_1$ and $\Omega_2$ by the interface $\Gamma := \bar{\Omega}_1 \cap \bar{\Omega}_2$, a multi-domain formulation of (2.14) can be written as

\[
\begin{array}{c|c}
\partial \Omega_1 \cap \partial \Omega & \\
\hline
\Omega_1 & -\Delta u_1 = f \quad \text{in } \Omega_1, \quad (2.15) \\
\Gamma & u_1 = 0 \quad \text{on } \partial \Omega_1 \cap \partial \Omega, \quad (2.16) \\
\Omega_2 & u_1 = u_2 \quad \text{on } \Gamma, \quad (2.17) \\
\partial \Omega_2 \cap \partial \Omega & \frac{\partial u_2}{\partial n} = \frac{\partial u_1}{\partial n} \quad \text{on } \Gamma, \quad (2.18) \\
\end{array}
\]

\[
\begin{array}{c|c}
\partial \Omega_2 \cap \partial \Omega & \\
\hline
\Omega_2 & u_2 = 0 \quad \text{on } \partial \Omega_2 \cap \partial \Omega, \quad (2.19) \\
\partial \Omega_2 \cap \partial \Omega & -\Delta u_2 = f \quad \text{in } \Omega_2, \quad (2.20) \\
\end{array}
\]

with the outer unit normal vector $n$ on $\Gamma$. The partial differential equation and the boundary conditions on the outer boundaries $\partial \Omega_1 \cap \partial \Omega$ and $\partial \Omega_2 \cap \partial \Omega$ correspond to the global problem (2.14). For the interface $\Gamma$, the so-called transmission or interface conditions (2.17) and (2.18) become necessary. The derivation of these conditions and the mathematical foundation of domain decomposition methods can be found in [24].
The decomposed problem \((2.15 - 2.20)\) can be solved by an iterative substructuring method. Here, the two subproblems are solved successively, starting from an initial guess \(u_0^1\) and \(u_0^2\). The algorithm creates two sequences of functions, \(\{u^1_k\}\) and \(\{u^2_k\}\), which converge towards the solutions \(u_1\) and \(u_2\). In order to solve the two subproblems separately in an iterative manner, an interface variable \(\lambda\) is needed to transfer the solution at the interface \(\Gamma\) from one subdomain to the other. Different choices for the boundary condition types on \(\Gamma\) are presented in [24], one of them being the Dirichlet-Neumann method:

Given \(\lambda^0\), solve for each \(k \geq 0\):

\[
-\Delta u^{k+1}_1 = f \quad \text{in } \Omega_1, \tag{2.21}
\]
\[
u^{k+1}_1 = 0 \quad \text{on } \partial\Omega_1 \cap \partial\Omega, \tag{2.22}
\]
\[
u^{k+1}_1 = \lambda^k \quad \text{on } \Gamma, \tag{2.23}
\]

then

\[
-\Delta u^{k+1}_2 = f \quad \text{in } \Omega_2, \tag{2.24}
\]
\[
u^{k+1}_2 = 0 \quad \text{on } \partial\Omega_2 \cap \partial\Omega, \tag{2.25}
\]
\[
\frac{\partial u^{k+1}_2}{\partial n} = \frac{\partial u^{k+1}_1}{\partial n} \quad \text{on } \Gamma, \tag{2.26}
\]

with

\[
\lambda^{k+1} := \theta u^{k+1}_2 \bigg|_{\Gamma} + (1 - \theta)\lambda^k, \tag{2.27}
\]

where \(\theta\) is a positive damping parameter. Equations \((2.23)\) and \((2.26)\) represent the Dirichlet and Neumann boundary conditions on \(\Gamma\) respectively.


Domain decomposition can be used for more complex homogeneous as well as heterogeneous problems. Some examples and generalizations are given in [24]. The next section applies the domain decomposition method to the special case of a Stokes/Darcy problem.

2.3 Iterative coupling for the Stokes/Darcy problem

The discretization of the mathematical model for the Stokes/Darcy problem derived in section 2.1 leads to a system of algebraic equations. Figure 2.1 shows two solution
strategies for such systems: The monolithic approach, where the global system is solved at once, and the domain decomposition approach, where the domain is split into subdomains with reduced systems which are solved successively. The global system matrix $A$ contains submatrices which belong to the free flow (blue) and porous medium (orange) subproblems. The gray submatrices $A_{\Gamma,ff}$ and $A_{\Gamma,pm}$ in figure 2.1a represent the entries of the global system matrix which resemble the coupling conditions. In the iterative approach, the solution of Darcy’s problem in the porous medium at the interface $\Gamma$ is used as a boundary condition for the Stokes problem at the lower boundary of $\Omega_{ff}$, and vice versa, see figure 2.1b.

Descriptions and numerical results for the monolithic approach can be found amongst others in [3] and [20]. Within this work, a domain decomposition technique is applied. The iterative algorithm is presented in the following, a mathematical analysis and the proof for well-posedness of the decomposed problem can be found in [13].

The iterative coupling method uses an interface equation for the separate solution of the two subdomains. For the Stokes/Darcy problem, two possibilities for the choice of the interface unknown $\lambda$ arise from the coupling conditions (2.12) and (2.10):

1. the trace of the pressure $p_{pm}$ on the interface, $\lambda = p_{pm} = p_{ff} + n \cdot ( -\varrho \nu \nabla v_{ff} ) n$, 

2. the trace of the normal velocity on the interface, $\lambda = v_{ff} \cdot n = ( -\frac{K}{\mu} \nabla p_{pm} ) \cdot n$.

The choice of $\lambda = v_{ff} \cdot n$ results in two Neumann boundary problems with respect to the interface $\Gamma$. As pointed out by [13], in contrast to the homogeneous case of a Poisson/Poisson coupling, two different boundary value problems are solved in the two subdomains in the heterogeneous case. In the following, $\lambda = v_{ff} \cdot n$ is used.

The iterative coupling algorithm for the Stokes/Darcy problem follows the same concept as the Poisson/Poisson algorithm in section 2.2. For transient problems, an outer
The current time $t$ is the sum of all previous time steps $\Delta t$. The superscript $i$ refers to the current time step, while the superscript $k$ belongs to the current iteration:

1. While $t < t_{\text{End}}$,
   
   2. choose an initial guess $\lambda^{0,i}$, for each $k \geq 0$
   
   3. solve Darcy’s problem (2.9) in $\Omega_{pm}$ with the continuity of normal fluxes (2.10) as a boundary condition on $\Gamma$,
   
   4. solve Stokes’ problem (2.3) and (2.8) in $\Omega_{ff}$ with the continuity of normal stresses (2.12) and the Beavers-Joseph-Saffman condition (2.13) as boundary conditions on $\Gamma$,
   
   5. update the interface variable $\lambda^{k+1,i} = \theta u^{k,i} + (1 - \theta) u^{k-1,i}$, where $u^{k,i} = (v^{k,i}_{ff}, p^{k,i}_{ff}, p^{k,i}_{pm})^T$ is the solution vector in the current iteration $k$,
   
   6. compute the residual $r$ over the whole domain $\Omega$, if $r > \varepsilon$ update $k := k + 1$ and go back to 3.
   
   7. update $t := t + \Delta t$ ($i := i + 1$), go back to 1.

The initial guess can be chosen as $\lambda^{0,i} = \lambda^{k,i-1}$ at the beginning of each time step. The pressure $p_{pm}$ computed in step 3 influences the Stokes subproblem via the boundary condition at the interface (2.12). The velocity $v_{ff}$ in the free-flow domain is transferred to the Darcy subproblem in the next iteration via the interface variable $\lambda$. Therefore, the two subdomains can be solved independently, but are still coupled to each other. The choice of the damping parameter $\theta \in (0, 1]$ to weight the influence of the previous solution and the solution of the Darcy subdomain in $\lambda$ affects the convergence behavior of the solution. According to [12], convergence can be reached only for certain values of $\theta$ in some cases.

The stationary version of the algorithm is obtained by dropping the time-dependent terms in the partial differential equations and omitting the outer time loop.

An alternative to the above described algorithm would be to use Robin boundary conditions at the interface. The behavior of such an approach is supposed to be more independent of the physical parameters $K$ and $\nu$. Implementing the Robin-Robin coupling method is however not possible with the software package used within this work, since the applied stencil is limited to one cell above and below the coupling.
interface respectively. For the computation of primary variable gradients, the values in the second row of cells would be necessary. Furthermore, the uncoupled residual of the porous medium subdomain $\Omega_{pm}$ is not available for the coupling method.

A multi-domain formulation for the coupled Navier-Stokes/Darcy problem is presented in [13] as well. In addition to the coupled Stokes/Darcy problem, a nonlinear extension operator is needed to derive the interface equation.

### 2.4 Additive Schwarz Preconditioned Inexact Newton

The iterative approach described in section 2.2 is an additive Schwarz method, which evolved from the alternating Schwarz method [25]. It solves smaller boundary value problems on the subdomains successively, then adds up the results to obtain the result for the global boundary value problem in the whole model domain.

Two possibilities to improve the additive Schwarz method are mentioned in [14]: either replacing the additive part by a multiplicative version, or replacing the Richardson iteration for $\lambda_{k+1}$ by an inexact Newton method. The second approach is the so-called additive Schwarz preconditioned inexact Newton (ASPIN) method.

A common approach to solve large sparse nonlinear systems of equations $F(u) = 0$ is the so-called inexact Newton method. The solution $u^*$ is computed with a fixed-point iteration of $F$. If the initial guess of $u$ is close enough to the solution, the iteration converges fast. In most cases, a good initial guess is difficult to obtain, especially for nonlinear equations. Therefore, the preconditioned inexact Newton method attempts to solve an equivalent nonlinearly preconditioned system $F'(u)p = 0$ instead of the original system $F(u) = 0$. The system is preconditioned such that it has the same solution $u^*$ as the original system, but less unbalanced nonlinearities. The preconditioned inexact Newton method is given as

1. Find $p^k$ such that

$$||F(u_k) - F'(u)p^k|| \leq \eta_k ||F(u_k)||,$$  \hspace{1cm} (2.28)

2. compute the new approximate solution

$$u^{k+1} = u^k - \lambda_k p^k.$$ \hspace{1cm} (2.29)

The vector $p^k$ represents the Newton direction. Its direction is determined in step 1,
while its magnitude is scaled in step 2 by $\lambda_k$. The theoretical determination of the step length parameter $\lambda_k$ and the constant $\eta_k$ is explained in [8].

Since the Jacobian $\mathcal{J} = \mathcal{F}'$ is a dense matrix, its computation and storage become expensive for large systems. The derivation in [8] yields the following formula for the Jacobian matrix of the preconditioned nonlinear system:

$$\mathcal{J} \approx \sum_{i=1}^{M} J_{S_i}^{-1} J,$$

(2.30)

where $J_{S_i}$ are the Jacobian matrices of the respective subsystems and $J$ is the Jacobian matrix of the original system.

With this approximation, the procedure for the ASPIN method is given by [8] as

1. Choose an initial guess $u^0$,

2. compute the nonlinear residual $\mathcal{F}(u^k) = g^k = \sum_{i=1}^{M} g^k_i$,

3. find the inexact Newton direction $p^k$ by solving

$$\sum_{i=1}^{M} J_{S_i}^{-1} J p^k = g^k$$

(2.31)

approximately, in the sense that $\|g^k - \sum_{i=1}^{N} J_{S_i}^{-1} J p^k\| \leq \eta_k \|g^k\|$

4. compute the new approximate solution $u^{k+1} = u^k - \lambda_k p^k$.

Step 2 contains the successive solution of the two subproblems and the subsequent calculation of the global residual. In the third step, pieces of the Jacobian matrix are computed, such that the full Jacobian matrix $\mathcal{J}$ does not have to be assembled. The new solution $u^{k+1}$ depends on the previous solution $u^k$ and the inexact Newton direction $p^k$, which is damped by a parameter $\lambda_k \in [0, 1)$. If the residual of the new solution is not yet sufficiently small, steps 2 to 4 are repeated for $k$ increased by one.

The analysis in [8] proves that the original nonlinear system $F(u) = 0$ and the nonlinearly preconditioned system $\mathcal{F}(u) = 0$ have the same solution $u^*$ under certain conditions. Local convergence and a convergence rate similar to that of the inexact Newton method are shown in [2].
3 Implementation

Several software packages are available for the numerical solution of partial differential equations. One of them is the Distributed and Unified Numerics Environment (DUNE, [1]), presented in section 3.1. The following sections explain the discretization of the Stokes/Darcy problem: Section 3.2 deals with the difficulties arising due to the structures of the subproblems, while section 3.3 explains the numerical method for the Stokes subdomain. The last sections describe the iterative coupling implementation (3.4) and the ASPIN implementation (3.5).

3.1 Software

DUNE is a modular toolbox which uses grid-based methods to solve partial differential equations. It is developed with a focus on generic programming techniques to obtain efficient and reusable code, which can easily be tailored to a specific need. One of its main principles is the separation of data structures and algorithms in order to facilitate maintenance and extension of the code. The DUNE core modules together with the add-on module dune-PDELab [5] and its extension dune-MultiDomain [21] provide the framework for the implementations within this thesis.

PDELab aims to simplify the implementation of discretization schemes for more realistic scenarios than test cases with analytical solutions. The generic programming approach enables the user to choose between various finite element function spaces, linear and nonlinear solvers, as well as explicit and implicit time discretizations. Combining these components as needed in a specific case substantially reduces the implementation time. The generic implementation enables to build simulation software with high performance as well as a high flexibility to adapt the software to a certain problem at the same time.

The PDELab programs usually solve single-physics problems. For the solution of multiphysics problems, such as the Stokes/Darcy problem, the extension MultiDomain is developed in [21]. With this extension, existing local operators for single-physics prob-
lems can be combined. Only the coupling conditions which describe the interactions between the subproblems have to be added by the user. A mechanism to subdivide the global spatial grid into subgrids corresponding to the subproblems is provided by MultiDomainGrid [21]. Using these two extension modules allows to easily switch between monolithic and iterative coupling without having to implement the multi-physics problem twice.

3.2 Discrete Stokes/Darcy problem

Discretizing sets of partial differential equations results in systems of the form \( Ax = b \), with the system matrix \( A \), the right-hand side \( b \) and the vector of unknowns \( x \). For the Darcy problem, this system is linear and can be solved with standard iterative solvers, such as the conjugate gradient solver and its modifications. The Stokes equations produce a nonlinear system with a block of zeros on the main diagonal of the system matrix. The solution \( x \) of the Stokes system is a saddle-point, which cannot be found by standard direct solvers. Solving discrete saddle-point problems poses a fundamental problem in scientific computing. Examples for saddle-point problem solvers are the direct solver SuperLU [19] and the iterative Uzawa-type solver presented amongst others in [6]. At the time of the preparation of this thesis, only an implementation of a direct solver was available.

Monolithically coupled Stokes/Darcy problems currently require the application of the direct solver for saddle-point problems in the whole model domain. By uncoupling the two subproblems and solving them independently, both subsystems can be treated according to their numerical behavior: A fast iterative solver is sufficient for the Darcy subproblem. At the same time, the expensive direct solver for the Stokes subproblem is applied to a smaller system compared to the monolithic approach. Exploiting these possibilities might reduce the computing time for Stokes/Darcy problems.

Figure 3.1a shows an example of the system matrix for the coupled Stokes/Darcy problem. This case is used to show the typical structure of such a matrix. Since each subdomain consists of four grid cells only, all entries correspond to boundary conditions and belong to primary unknowns in boundary cells. Therefore, the matrix is not symmetrical and the entries differ along the diagonal, even though the corresponding problem is diffusion-dominated. As shown by the coloring, the matrix is sparse since most entries are zero (medium blue). The entries in the upper left block correspond to the Stokes subproblem, the lower right block resembles the Darcy subproblem. Entries (7,19), (8,20), (19,7) and (20,8) result from the coupling conditions. The Stokes matrix for the decomposed approach is shown in figure 3.1b. The zero entries on the main
diagonal reflect the saddle-point property of the Stokes problem. The corresponding Darcy matrix is given in figure 3.1c.

### 3.3 MAC scheme

An alternative to standard finite element methods for the solution of incompressible Navier-Stokes equations is presented in [16]. The so-called marker-and-cell (MAC) scheme uses a staggered grid: Instead of defining all primary variables in the cell centers, the velocity components are moved to the cell boundaries. As depicted in figure 3.2, the horizontal velocity component $u$ is computed at the vertical cell boundaries, while the vertical component $v$ is set on the horizontal cell boundaries. The pressure remains in the cell centers, which are numbered with integer indices. Boundaries, such as rigid walls, coincide with the respective cell boundaries. For a horizontal wall, all vertical velocity components $v$ on the wall become zero, while the horizontal components $u$ are computed with the help of velocity components $u'$ from outside cells. This applies to vertical walls vice versa. The respective boundary conditions for velocity and pressure are derived in [17].

The analysis in [22] proves the convergence of the discrete approximations to the exact solutions for the stationary Stokes equations and yields error estimates for the pressure and the velocity. The corresponding pressure error estimates for the Navier-Stokes equations are obtained in [23].

For multi-domain problems, the coupling interface should coincide with the cell boundaries of the interface grid cells. The implementation for this thesis uses a staggered grid for the Stokes subdomain and a cell-centered finite volume method for the Darcy
The boundary condition for the porous medium is the continuity of normal fluxes \( (2.10) \). Since the free flow velocity \( v_{ff} \) is computed at the pressure cell boundary which coincides with the interface, it can be directly used as a boundary condition for the porous medium.

The remaining two boundary conditions are adapted to the staggered grid in the free flow subdomain. For the continuity of normal stresses, the pressure in the porous medium \( p_{pm} \) as well as the lower half of the free flow cell at the interface are taken into account, see figure 3.3a. The Beavers-Joseph-Saffman condition \( (2.13) \) has to be split between two half cells, which divide the grid cell vertically. Figure 3.3b shows the tangential velocity components on the left and the right edge of a grid cell, whose influences are added up by the coupling operator.
3.4 Iterative coupling method

An iterative coupling approach to compute the Poisson/Poisson problem with a cell-centered finite volume method is implemented in [1]. A monolithic coupling operator for the Stokes/Darcy problem with a staggered grid discretization has already been developed at the Department of Hydromechanics and Modelling of Hydrosystems. These two approaches are now combined to an iterative coupling method for the Stokes/Darcy problem on a staggered grid. The algorithm for stationary problems is extended in order to handle transient problems as well.

The implemented iterative algorithm differs from the algorithm presented in [13] (see section 2.3). Due to slightly better results with respect to computing time and convergence behavior, the Stokes subproblem is solved first. Therefore, the interface variable is chosen as $\lambda = p_{\text{pm}}$ and updated after the computation of the Darcy subdomain. The iteration is stopped if one of the following abort criteria is fulfilled:

\begin{itemize}
  \item $\frac{\text{residual}}{\text{start residual}} < \text{relative reduction},$
  \item $\text{residual} < \text{maximum error},$
  \item $\text{number of iterations} \geq \text{maximum number of iterations}.$
\end{itemize}

The quantities on the right hand sides as well as the damping parameter $\theta$ can be set by the user via a parameter file. Underlying structures such as the grid, grid function spaces, local operators and boundary conditions are identical for the monolithic and the iterative coupling approach.

Splitting the global problem into two subproblems is realized by using the respective submatrices instead of the global system matrix. In contrast to the monolithic approach, only the Stokes matrix is handed over to the solver in the Newton method. The Darcy matrix is handled by an iterative solver. Giving the correct matrices to the respective solvers is crucial and can only be achieved if the coupling operator does not inherit from any fully coupled operators. Additionally, all operations on neighbor matrices of the current matrix have to be omitted in the decomposed approach. Otherwise, the coupling operator might try to operate on the nonexistent coupling matrices ($A_{\Gamma,ff}$, $A_{\Gamma,pm}$ in figure 2.1a). This applies especially to the coupling of the Jacobian matrices, where self-self, self-neighbor, neighbor-self and neighbor-neighbor terms are accumulated in the monolithic version of the Stokes/Darcy coupling. For the independent solution of the Stokes subproblem this includes again all operations on the Darcy submatrix and the coupling matrices $A_{\Gamma,ff}$ and $A_{\Gamma,pm}$. In addition, the coupling of the Jacobian matrices is restricted to the Stokes subproblem. Furthermore, the coupling
3.5 ASPIN method

operator is not supposed to change any entries in the Darcy matrix when solving the Stokes’ problem, and vice versa.

Another difference to the monolithic approach is the application of the coupling conditions. The monolithic approach includes all three coupling conditions in the global system matrix. Following the algorithm presented in section 2.3, the iterative approach picks the coupling conditions according to the currently solved subproblem. A coupling mode is attached to each subproblem and used by the coupling operator to decide which of the coupling conditions have to be applied: (2.10) for the Darcy subproblem or (2.12 and 2.13) for the Stokes subproblem respectively.

For transient problems, the underlying implementation of the Stokes subproblem is switched to a transient MAC scheme. The storage terms are added for both subproblems and an integration over time is carried out. The iterative coupling operator does not change, but a time loop over the whole iterative algorithm in section 2.3 is added as indicated. Additionally, the abort criterion is extended in a way such that at least one iteration is done in each time step. Otherwise, the first or second criterion can possibly be fulfilled already due to the residual calculations in the previous time step.

The DUNE core module dune-istl [7] offers a variety of solvers which can be swapped easily. Within this work, a Newton method with a direct solver (SuperLU, [9]) solves the Stokes subproblem in the upper subdomain. A linear solver consisting of a preconditioner (Symmetric successive overrelaxation) and an iterative solver (Biconjugate gradient stabilized solver) is applied to the Darcy subproblem. The monolithic coupling applies a Newton method with a direct solver (SuperLU) to the global system.

3.5 ASPIN method

Since the domain decomposition which is applied in the iterative coupling method in section 2.3 is already a preconditioning technique, only the inexact Newton method has to be incorporated into the existing algorithm in order to obtain the ASPIN method described in section 2.4. The implementation of the first step, computing the global nonlinear residual, can be adopted from the existing implementation.

For the special case of two nonoverlapping subdomains, the approximate Jacobian of the preconditioned system \( \mathbf{J} \) (2.30) is given as

\[
\mathbf{J} = \sum_{i=1}^{2} J_{S_i}^{-1} \mathbf{J} = \begin{pmatrix} I & J_{11}^{-1} J_{12} \\ J_{22}^{-1} J_{21} & I \end{pmatrix},
\]

(3.1)
where $I$ is the identity matrix. With this formulation, equation (2.31) results in a linear system of equations

\[
\begin{pmatrix}
I & J^{-1}J_{12} \\
J_{22}^{-1}J_{21} & I
\end{pmatrix}
\begin{pmatrix}
p_{1}^k \\
p_{2}^k
\end{pmatrix} =
\begin{pmatrix}
g_1 \\
g_2
\end{pmatrix}.
\]

(3.2)

The new inexact Newton direction can then be computed in an iterative manner as

\[
p_{1}^l = g_1 - J^{-1}_{11}J_{12}p_{2}^{l-1},
\]

(3.3)

\[
p_{2}^l = g_2 - J^{-1}_{22}J_{21}p_{1}^{l-1}
\]

(3.4)

for $l = 1, ..., l_{\text{max}}$ and an initial guess $p^0$.

Since the Stokes/Darcy problem consists of two nonoverlapping subdomains, this simplified algorithm is implemented in the following. The matrix $J_{11}$ corresponds to the Stokes matrix, $J_{22}$ is the Darcy matrix, and the coupling matrices are denoted as $J_{12}$ and $J_{21}$. Due to the separate solution of the two subproblems, the global Jacobian matrix $J$ is never assembled for the iterative coupling approach. Therefore, its submatrices $J_{12}$ and $J_{21}$ are not available in the implementation.

**Step 2: Find the inexact Newton direction**

A way to work around the unavailability of $J_{12}$ and $J_{21}$ has to be found. It might be possible to obtain the coupling matrices by setting up the global system matrix separately, but this approach would require extra computing effort. Another possibility could be to compute the inexact Newton direction $p^k$ as the residual $\Delta u^k$ via

\[
J \underbrace{\Delta u^k}_{p^k} = F(u^k),
\]

(3.5)

corresponding to the general idea of an inexact Newton method. This approach results in a system of equations

\[
\begin{pmatrix}
J_{11}p_{1}^k + J_{12}p_{2}^k \\
J_{21}p_{1}^k + J_{22}p_{2}^k
\end{pmatrix} =
\begin{pmatrix}
F_1(u^k) \\
F_2(u^k)
\end{pmatrix}.
\]

(3.6)

The matrices $J_{12}$ and $J_{21}$ can be avoided by transforming (3.6) to

\[
J_{12}^{-1}p_{2}^{l-1} = F_1(u^k) - J_{11}p_{1}^l,
\]

(3.7)

\[
J_{21}^{-1}p_{1}^{l-1} = F_2(u^k) - J_{22}p_{2}^l.
\]

(3.8)
and using the results as right-hand sides for the following linear systems of equations:

\[ J_{11} x_1 = J_{12} p_{l-1}^1, \]  
\[ J_{22} x_2 = J_{21} p_{l-1}^2. \]  

(3.9)  
(3.10)

After solving this system for \( x \), the new inexact Newton direction can be calculated via equations (3.3, 3.4). The initial guess \( p^0 \) is set to zero in each outer iteration \( k \). The computation of \( p^k \) is done iteratively, for an iterator \( l \) up to a given number of iterations \( l_{\text{max}} \). Therefore, the expensive computations which would be necessary to check the abort criterion suggested by [8] are omitted. By testing the algorithm for different values of \( l_{\text{max}} \), a value which delivers sufficiently accurate solutions is determined.

**Step 3: Compute the new approximate solution**

A costly way to compute \( \lambda_k \) in each iteration is given in [8]. The following procedure shows a simpler alternative:

1. Compute the new solution \( u^{k+1} = u^k - \lambda_k p^k \) and its residual \( F(u^{k+1}) \),
2. if \( \|F(u^{k+1})\| > \|F(u^k)\| \), set \( \lambda_k = 0.5\lambda_k \) and go back to 1.,
3. if \( \|F(u^{k+1})\| \leq \|F(u^k)\| \), use \( u^{k+1} \) as the solution for the current iteration \( k \),
4. proceed with the next outer iteration \( k + 1 \).

To avoid \( \lambda \) to become too small without improving the overall solution, a limit such as \( 1/16 \) or \( 1/32 \) can be set.
4 Numerical results

The algorithms presented in sections 2.2, 2.3 and 2.4 are now applied to different test cases. Several grid refinements are performed to examine the convergence of the $L_2$ errors for test cases with known solutions. The previous implementation of a monolithic coupling method allows to compare its computing times with the iterative coupling implemented in this work. The following sections present numerical results for the Poisson/Poisson problem (4.1), the stationary (4.2) and transient (4.3) Stokes/Darcy problem, as well as for the ASPIN algorithm (4.4).

4.1 Poisson/Poisson problem

Further numerical experiments with the iterative coupling method for the cell-centered Poisson/Poisson problem implemented in [1] are carried out in this section. Two test cases with given solutions are set up. The right-hand sides $f$ are computed by inserting the respective given solution $u$ into the Poisson equation $-\Delta u = f$, see table 4.1. Then, the Dirichlet boundary conditions are set according to $u$, while the sink/source term is given by $f$. Therefore, the exact and approximate solutions can be compared by computing the $L_2$ error. Up to ten grid refinements are performed, leading to $1024 \times 1024 = 1048576$ grid cells per subdomain. Due to the cell-centered discretization, this number represents the degrees of freedom in each subdomain. For the sake of simplicity, the density $\rho$ and the kinematic viscosity $\nu$ are set to 1.

$$
\begin{array}{c|c}
\hline
u & f \\
\hline
3x^3 + 2y^3 - 5x^2y^2 & 10x^2 + 10y^2 - 18x - 4 \\
e^{-y} + x^3 & -e^{-y} - 6x \\
\hline
\end{array}
$$

Table 4.1: Test cases for the Poisson problem $-\Delta u = f$. 
Convergence

Figure 4.1 shows the $L_2$ errors for the two test cases. The convergence behavior meets the expectations since the $L_2$ errors decrease with a rate of $O(n^2)$, where $n$ is the reciprocal of the number of cells per space dimension. The monolithic coupling method delivers the same results.

Computing times

The computations for different grid refinements are each carried out five times and arithmetically averaged to obtain representative computing times. Figure 4.2 presents the ratio of the computing times needed by the monolithic and the iterative coupling method for the same problem. The very high ratios for one grid refinement are omitted since a grid of four grid cells is not significant for realistic applications. A ratio larger than 1.0 is reached if the iterative method is faster than the monolithic method. According to these results, the iterative method pays off for high resolutions, even though the same linear solvers are used in both subdomains. For example, computing the second test case with ten grid refinements takes approximately 2 hours and 13 minutes with the monolithic coupling, compared to approximately 33 minutes for the iterative approach. These outcomes are a further motivation to investigate the iterative coupling method for heterogeneous problems such as the Stokes/Darcy problem.
The damping parameter $\theta \in (0, 1]$ weights the influence of the solutions in the previous and the current iteration $k$:

$$\lambda^{k+1} = \theta u^k + (1 - \theta) u^{k-1}.$$  \hspace{1cm} (4.1)

According to [24], a damping parameter $\theta < 1.0$ is usually needed to guarantee convergence or to accelerate the solution process. A parameter value of 0.7 is used in [12] for the coupled Stokes/Darcy problem.

The numerical experiments in [1] yield an optimal damping parameter $\theta_{opt} = 1.0$ for a coupled Poisson/Poisson problem. Due to deviating results in the literature, further investigations are made within this work to rule out any implementation errors.

The iterative coupling method for a Poisson/Poisson problem implemented in [21] is used as a reference in the following. This implementation uses either $Q_1$ or discontinuous Galerkin $Q_2$ elements for the discretization, while $P_0$ elements are used in the implementation in [1]. Two test problems are computed with these two different implementations. The simple problem is taken out of [1]: only Dirichlet boundary conditions are set, no sinks or sources occur and the interface divides the two squared subdomains horizontally, see figure 4.3a. The complex problem is implemented in [21] and has a source term, Neumann boundary conditions, more complex functions for the Dirichlet boundaries and a vertical interface as shown in figure 4.3b.
4.1 Poisson/Poisson problem

Figure 4.3: Setups to determine the optimal damping parameter for the Poisson/Poisson problem ($\mathbf{x} = (x, y)^T$).

<table>
<thead>
<tr>
<th>Problem</th>
<th>$P_0$</th>
<th>$Q_1$</th>
<th>DG $Q_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple (fig. 4.3a)</td>
<td>1.0</td>
<td>1.0</td>
<td>0.95</td>
</tr>
<tr>
<td>Complex (fig. 4.3b)</td>
<td>1.0</td>
<td>0.81</td>
<td>0.81</td>
</tr>
</tbody>
</table>

Table 4.2: Optimal damping parameters $\theta_{\text{opt}}$ for different implementations.

Both problems are computed with their original implementation as well as with the respective other implementation. A variation of the damping parameter $\theta$ is carried out for both problems with the three different finite element types. The results for the optimal damping parameter concerning the accuracy of the solution and the computing time are listed in Table 4.2. The optimal damping parameter for the complex problem with $Q_1$ or discontinuous Galerkin $Q_2$ elements matches the results found in the literature. However, using the $P_0$ elements of a lower order results in an optimal damping parameter of $\theta_{\text{opt}} = 1.0$ for the complex problem, which supports the author’s results in [1]. This result suggests that the optimal damping parameter values depend on the computed problem and its discretization. The discretization based on $P_0$ elements needs less iterations to obtain the same results as the discretizations with $Q_1$ and $Q_2$ elements. Furthermore, the $P_0$ discretization produces the smallest $L_2$ errors.
4.2 Stationary Stokes/Darcy problem

The model domain $\Omega \in \mathbb{R}^2$ for the Stokes/Darcy problem consists of the two subdomains $\Omega_{\text{ff}} = (0, 1) \times (1, 2)$ and $\Omega_{\text{pm}} = (0, 1) \times (0, 1)$, with the interface $\Gamma = (0, 1) \times \{1\}$. The boundary condition types are given in figure 4.4a. The MAC scheme (see section 3.3) is used for the spatial discretization in the free flow subdomain.

The iterative coupling method is applied to four test cases with analytical solutions. The test cases differ in the direction of flow given at the Dirichlet boundary, the presence of a pressure jump at the interface and sink/source terms for mass and momentum. The corresponding values can be found in table 4.3. In the following, the boundary condition values and sink/source terms of the first case are derived to match the given solutions.

For vertical flow, the horizontal velocity component is set to zero according to the Beavers-Joseph-Saffman condition (2.13):

$$0 = v_x + \frac{\partial}{\partial y} v_x \quad \Rightarrow \quad v_x = 0 \quad \Rightarrow \quad v_{\text{ff}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (4.2)$$

The vertical velocity component $v_y$ needs to be non-zero and is set to 1 for simplicity. The coupling condition for the normal velocities (2.10) yields the Dirichlet boundary
4.2 Stationary Stokes/Darcy problem

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>(v_x)</td>
<td>0</td>
<td>(e^{-y})</td>
<td>0</td>
<td>100(e^{-y})</td>
</tr>
<tr>
<td>(v_y)</td>
<td>1</td>
<td>0</td>
<td>(y)</td>
<td>2(y)</td>
</tr>
<tr>
<td>(p_{ff})</td>
<td>(-y)</td>
<td>7</td>
<td>(-y + 7)</td>
<td>(-2y + 6)</td>
</tr>
<tr>
<td>(p_{pm})</td>
<td>(-y)</td>
<td>7</td>
<td>(-y + 6)</td>
<td>(-2y + 4)</td>
</tr>
<tr>
<td>(q_{\text{mom},x})</td>
<td>0</td>
<td>(-e^{-y})</td>
<td>0</td>
<td>(-100e^{-y})</td>
</tr>
<tr>
<td>(q_{\text{mom},y})</td>
<td>-1</td>
<td>0</td>
<td>-1</td>
<td>2</td>
</tr>
<tr>
<td>(q_{\text{mass},ff})</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>(q_{\text{mass},pm})</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 4.3: Values for Dirichlet boundaries and sink/source terms \(q\).

condition value for the pressure \(p_{pm}\) in the Darcy subdomain as

\[
\frac{\partial}{\partial y} p_{pm} = -v_y = -1 \quad \Rightarrow \quad p_{pm} = -y. \tag{4.3}
\]

The Dirichlet boundary condition value for the Stokes pressure \(p_{ff}\) is obtained with the first coupling condition \([2.12]\):

\[
p_{pm} = p_{ff} - \frac{\partial}{\partial y} v_y = p_{ff} - \frac{\partial}{\partial y} 1 \quad \Rightarrow \quad p_{pm} = p_{ff} = -y. \tag{4.4}
\]

The source terms are the results of the balance equations for mass and momentum. For the Stokes subdomain, they are

\[
\nabla \cdot (\rho \mathbf{v}_{ff}) = 0 = q_{\text{mass},ff}, \tag{4.5}
\]

\[
\nabla \cdot (-\rho \nu \nabla \mathbf{v}_{ff}) + \nabla p_{ff} = 0 + \begin{pmatrix} 0 \\ -1 \end{pmatrix} = q_{\text{mom}}. \tag{4.6}
\]

The mass source term in the Darcy subdomain is obtained with

\[
\nabla \cdot \left( -\frac{K}{\mu} \nabla p_{pm} \right) = 0 = q_{\text{mass},pm}. \tag{4.7}
\]

A damping parameter \(\theta = 1.0\) delivers the fastest results, see section \([4.2.1\)] and is therefore used in the following computations. If not stated otherwise, the error tolerance for the relative reduction is set to \(\varepsilon = 10^{-8}\). The number of grid refinements \(r\) corresponds to the number of grid elements per space dimension \(m\) via \(m = 2^r \cdot 2^r\). Figure \([4.4b]\) shows the pressure solution and the streamlines representing the velocity field of test case D for 5 grid refinements.
4.2.1 Damping parameter

For the stationary test cases within this work, the $L_2$ error does not change significantly with the damping parameter $\theta$. In general, the $L_2$ errors decrease for $\theta \to 1.0$.

The investigation of the influence on the computing times for all four test cases shows that the optimal damping parameter can be found in the interval $[0.95, 1.0]$ in all four test cases. For 1024 grid cells in each subdomain, the smallest computing times and $L_2$ errors are achieved with $\theta_{\text{opt}} = 0.98$, see figure 4.5. For $\theta = 1.0$, only one additional iteration is necessary, which adds less than 1 second to the total computing time in these cases. Refining the grid further leads to optimal damping parameters of $\theta_{\text{opt}} = 1.0$. Due to the very small differences, a damping parameter of $\theta = 1.0$ is chosen for the solution of all test cases within this work.

4.2.2 Convergence

By setting the boundary condition values as given in table 4.3 the $L_2$ error can be computed. Figure 4.6 shows the results for eight grid refinements, test case D is only computed for seven refinements since the Newton solver in the monolithic coupling method does not converge for eight refinements. The $L_2$ error decreases with the expected rate of $n^2$, where $n = 1/m$. The high convergence rate of the velocity $L_2$ error (figure 4.6a) might be caused by the simple set up of test case A. The same $L_2$ errors are obtained with the monolithic coupling method.
4.2 Stationary Stokes/Darcy problem

4.2.3 Computing time

The computing times needed for the test cases A, B, C and D in section 4.2.2 are measured five times for both coupling methods. The arithmetically averaged values of $t_{\text{iter}}/t_{\text{monot}}$ are compared in figure 4.7. A ratio larger than 1 means that the iterative method is faster than the monolithic method. Such ratios are expected due to the theoretically faster solution with the iterative coupling, see section 2.3. The tests show that the iterative method cannot overtake the monolithic method for the stationary test cases examined within this work. Further measurements show that the Newton method in the iterative approach needs almost the same time for the solution of the Stokes subproblem as the Newton method in the monolithic approach needs for the solution of the global system. Since the Stokes problem is solved several times in the iterative method, the total computing time is accordingly higher.
With the previously described problem settings and parameter values, six iterations are necessary to obtain the same $L_2$ errors as the monolithic method. In order to reduce the iterative computing time, less iterations as well as a faster solution of the Stokes subproblem would be necessary. With the current implementation, such improvements are impossible without a deterioration of the solution’s accuracy. Neither changing the position nor the length of the interface influences the computing times such that the iterative coupling becomes the faster method. For stationary Stokes/Darcy problems with up to $4^8$ grid elements, the monolithic coupling method seems to be the better choice. The increase of $\frac{t_{\text{mono}}}{t_{\text{iter}}}$ with higher grid refinements might lead to values larger than 1 for higher numbers of grid elements or larger problems.

### 4.2.4 Parameter variation

Varying the values of the intrinsic permeability $K$ or the kinematic viscosity $\nu$ shows the weakness of the currently implemented iterative coupling method. While the monolithic algorithm still converges for steady cases with small values of $K$, the iterative algorithm fails for $K \leq 0.01$. Therefore, no realistic values for $K$ can be used with the current iterative method. The same difficulties for small $K$ and $\nu$ are observed by [10]. An approach to improve the iterative method is made in [11] by using Robin boundary conditions for both subproblems at the interface $\Gamma$. The resulting algorithm which does still converge for small entries of $K$ and small values of $\nu$ is given in [11]. Since it was not possible to implement this Robin-Robin coupling method into the existing implementation, the application of the iterative coupling method is currently restricted to nonrealistic examples.
4.3 Transient Stokes/Darcy problem

4.3.1 Analytical test cases

The model domain and test cases in section 4.2 are used to solve the transient equations as well. The Dirichlet boundary condition values for the velocity in the upper subdomain are modified to be time-dependent by multiplication with the factor $\sin^2(t)$. Since $\sin^2(\pi/2) = 1$, the exact solution of the transient problems is consistent with the one for the stationary test cases for $t_{\text{end}} = \pi/2$. The time step size is set to be $\Delta t = \pi/20$ and an implicit Euler method is applied for the temporal discretization. In contrast to the stationary test cases, the iterative algorithm does not fail for $K \leq 0.01$. Therefore, simulations with more realistic values such as $K = 10^{-8}$ are feasible. Testing the transient problems for optimal damping parameters leads to $\theta_{\text{opt}} = 1.0$, which is therefore used in the following computations.

Convergence

Figure 4.8 shows the $L_2$ errors for six refinements for the transient test case D. For the transient test cases, the grid cell length as well as the time step size are halved with each refinement. Even though the $L_2$ errors are relatively high for all three primary variables, they converge towards the exact solution with decreasing grid element sizes and a convergence rate of $O(n^2)$ with $n = 1/m$. Similar results are obtained for the other three transient test cases as well.

4.3.2 Application-driven problem

A test case E without known analytical solution is used to determine the performance for more realistic scenarios. The same parameter values for solvers and error tolerances are used as in the previous analytical examples. The boundary condition types and values are given in figure 4.9a, no sinks or sources occur. The test case models a parabola-shaped velocity profile at the left free flow boundary, a pressure gradient in the porous medium and a central lens with a lower permeability than in the surrounding porous medium. In this case, the permeability is set to $K = 10^{-5}$ in the permeability lens and to $K = 10^{-1}$ in the remaining porous medium. Figure 4.9b shows the resulting pressure solution and the streamlines representing the velocity field for the iterative coupling method with $\Delta t = 16 \cdot \pi/20$ and $t_{\text{end}} = 16 \cdot \pi/2$. 
Figure 4.8: $L_2$ errors for six grid refinements for test case D (transient).

Figure 4.9: Setup and result for test case E.
Computing times

In order to compare the iterative method with the monolithic approach, the computing times are measured five times and arithmetically averaged. The resulting computing time ratios are displayed in figure 4.10. Again, a trend towards a ratio of 1 shows the further potential of the iterative method for high resolutions and/or large numbers of degrees of freedom. The computing time ratios for the transient problem are higher than the ratios for the stationary analytical test cases in section 4.2.

4.4 ASPIN method

The convergence behavior of the ASPIN method for decreasing grid element sizes is examined by performing seven grid refinements and computing the respective $L_2$ errors. The results for the stationary test case D from section 4.2 are shown in figure 4.11. Similar results are obtained for the other stationary test cases, which all yield convergence rates of $O(n^2)$ for the three primary unknowns.

Since the ASPIN method needs approximately twice the computing time of the standard iterative method in section 4.2, an attempt to improve the computing times is made. One possible approach is to scale the inexact Newton direction already before using it to compute the new approximate solution. Therefore, equations (3.3) and (3.4)
for \( l = 1, \ldots, l_{\text{max}} \), an initial guess \( p^0 \) and a damping parameter \( \Theta \in [0, 1] \). A damping parameter \( \Theta = 1 \) corresponds to the ASPIN method described in sections 2.4 and 3.5. The results of a variation of \( \Theta \) are given in figure 4.12. The \( L_2 \) errors are almost identical, but the global residual strongly depends on \( \Theta \). The higher the global residual, the higher the number of necessary iterations to reach the given error tolerance of \( 10^{-8} \). The optimal parameter value concerning the number of iterations and therefore the computing time is \( \Theta = 0 \). This choice of \( \Theta \) corresponds to the standard iterative coupling method applied in section 4.2 since the global solution obtained by the successive solution of the subdomains is then used without further modifications. The results obtained in the numerical experiments match these expectations. Therefore, the ASPIN method does not improve the standard iterative method for the stationary test cases.

In the previous calculations, the iteration to obtain the new inexact Newton direction (3.3) (3.4) is carried out once with \( l_{\text{max}} = 1 \). Choosing \( l_{\text{max}} > 1 \) results in higher numbers of iterations needed to obtain a sufficiently small global residual, although calculating the inexact Newton direction iteratively is supposed to deliver better results. A possible explanation for this behavior could be that the approach to bypass the coupling matrices \( J_{12} \) and \( J_{21} \) is not correct.
The ASPIN method was found to be very robust for problems with high Reynolds numbers by [14]. Applying the iterative coupling method to coupled Navier-Stokes/Darcy problems would allow to compute such problems and compare the results of the standard iterative method and the ASPIN method.
5 Summary and conclusion

Interactions between a free flow and an adjacent porous medium flow are part of many technical and environmental processes. Modeling such interactions requires a numerical multi-domain model equipped with a coupling method to exchange data between the two subproblems. The theory of domain decomposition methods motivates the application of an iterative coupling approach as an alternative to monolithic coupling. Exploiting the separate solution of the subproblems is expected to reduce the computing times and therefore allow the simulation of large systems modeling realistic application scenarios.

Within this work, an iterative coupling method for the coupled Stokes/Darcy problem is implemented. This algorithm is applied to stationary as well as transient test cases and can thus be compared to the monolithic coupling method. Furthermore, the ASPIN method is implemented as a modified version of the iterative coupling approach.

The iterative coupling method is examined further for a Poisson/Poisson problem to supplement the investigations in [1]. A satisfying convergence behavior and an optimal damping parameter of $\theta = 1$ can be confirmed. For the Stokes/Darcy problem, four test cases with analytical solutions demonstrate the convergence behavior of the iterative coupling method for increasing numbers of grid elements. A convergence rate of $O(n^2)$ is reached for all unknowns with both the stationary and transient problems. Since the monolithic coupling method obtains the same rates, the computing times of the two coupling methods are compared. For the stationary test cases, the monolithic method is at least three times faster than the iterative coupling method, despite applying a fast iterative solver to the Darcy subproblem. Considering the growth of the computing time ratios for increasing grid refinements, the iterative method seems to pay off for high resolutions only. A transient test case without a known solution yields higher computing time ratios, but the iterative method does not overtake the monolithic method for seven grid refinements. The ASPIN approach yields the same convergence behavior as the original iterative coupling method, but needs twice the computing time to obtain the same accuracy. Further experiments show that the ASPIN method does not deliver more accurate results for stationary test cases than the original iterative method.
The numerical experiments show that the same accuracy can be reached with both the monolithic and the iterative coupling approach. Due to the size of the local Stokes matrix compared to the global Stokes/Darcy matrix, the iterative coupling method will probably be faster than the monolithic method for high grid resolutions or large problems in general. Furthermore, the iterative approach could be useful for problems with larger Darcy subdomains or more complicated models for the porous medium flow, which both result in larger Darcy matrices. Modeling application scenarios usually demands high numbers of degrees of freedom which result in large systems of equations. The current results imply that the iterative method could be an alternative to the monolithic approach for such cases. For one-phase problems such as the ones examined in this work, the effort of the iterative coupling method does not pay off. This might change for two-phase or nonisothermal two-phase problems, because more nonlinearities occur and more Newton iterations become necessary with the monolithic approach. Solving the Stokes subproblem separately would reduce the cost of these iterations. Since the convergence behavior of the iterative coupling method for such problems is uncertain, it has to be tested by numerical experiments. Furthermore, the computing times are only expected to decrease significantly if the subproblem solvers are improved, e. g. by implementing an iterative solver for the Stokes subproblem.

The findings within this work open up a range of possibilities for future implementations within the DUNE framework. Faster computing times could be obtained by the implementation of an iterative solver which can handle the saddle-point structure of the Stokes subproblem. Having faster solvers for the subproblems seems to be a promising way to achieve a computing time reduction compared to the monolithic method. For coupled problems with larger Darcy subdomains, the iterative method might overtake the monolithic method with the currently implemented solvers.

For transient problems, the sequential solution of the two subdomains allows the use of different time steps, depending on the occurring velocities in the respective subdomain. A criterion for the time step sizes and the frequency of an exchange of the variables’ values would then become necessary. Further exploitation of the separate solution could be the use of different grid cells, provided that a potential unconformity at the interface is handled correctly. More robust algorithms could be obtained by following up the implementation of Robin-Robin boundary conditions at the interface as suggested in [11] to tackle low permeabilities, or the ASPIN method for high Reynolds numbers in coupled Navier-Stokes/Darcy problems.
Bibliography


**Published Preprints**

http://www.nupus.uni-stuttgart.de

<table>
<thead>
<tr>
<th>Year</th>
<th>Authors</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>2007/1</td>
<td>Cao, Y. / Eikemo, B. / Helmig, R.</td>
<td>Fractional flow formulation for two-phase flow in porous media</td>
</tr>
<tr>
<td>2007/2</td>
<td>Korteland, S.-A.</td>
<td>The average equilibrium capillary pressure-saturation relationship in two-phase flow in porous media</td>
</tr>
<tr>
<td>2008/1</td>
<td>Helmig, R. / Weiss, A. / Wohlmuth, B.</td>
<td>Variational inequalities for modeling flow in heterogeneous porous media with entry pressure</td>
</tr>
<tr>
<td>2008/2</td>
<td>Cao, Y. / Helmig, R. / Wohlmuth, B.</td>
<td>Convergence study and comparison of the multipoint flux approximation L-method</td>
</tr>
<tr>
<td>2008/3</td>
<td>van Duijn, C.J. / Pop, I.S. / Niessner, J. / Hassanzadeh, S.M.</td>
<td>Philip's redistribution problem revisited: the role of fluid-fluid interfacial areas</td>
</tr>
<tr>
<td>2008/4</td>
<td>Niessner, J. / Hassanzadeh, S.M.</td>
<td>Modeling kinetic interphase mass transfer for two-phase flow in porous media including fluid–fluid interfacial area</td>
</tr>
<tr>
<td>2008/5</td>
<td>Niessner, J. / Hassanzadeh, S.M.</td>
<td>A model for two-phase flow in porous media including fluid–fluid interfacial area</td>
</tr>
<tr>
<td>2008/6</td>
<td>Cao, Y. / Helmig, R. / Wohlmuth, B.</td>
<td>Geometrical interpretation of the multipoint flux approximation L-method</td>
</tr>
<tr>
<td>2008/7</td>
<td>Vervoort, R.W. / van der Zee, S.E.A.T.M.</td>
<td>Simulating the effect of capillary flux on the soil water balance in a stochastic ecohydrological framework</td>
</tr>
<tr>
<td>2008/8</td>
<td>Niessner, J. / Hassanzadeh, S.M.</td>
<td>Two-phase flow and transport in porous media including fluid–fluid interfacial area</td>
</tr>
<tr>
<td>2008/10</td>
<td>Wolff, M.</td>
<td>Comparison of mathematical and numerical models for two-phase flow in porous media</td>
</tr>
<tr>
<td>2008/11</td>
<td>Darcis, M.</td>
<td>Implementation of a numerical model for the convection-enhanced delivery of therapeutic agents into brain tumors</td>
</tr>
<tr>
<td>2008/12</td>
<td>Cao, Y. / Helmig, R. / Wohlmuth, B.</td>
<td>Convergence of the multipoint flux approximation L-method for homogeneous media on uniform grids</td>
</tr>
<tr>
<td>2008/13</td>
<td>Ochs, S.O.</td>
<td>Development of a multiphase multicomponent model for PEMFC</td>
</tr>
<tr>
<td>2008/14</td>
<td>Walter, L.</td>
<td>Towards a model concept for coupling porous gas diffusion layer and gas distributor in PEM fuel cells</td>
</tr>
<tr>
<td>2009/1</td>
<td>Hægland, H. / Assteerawatt, A. / Helmig, R. / Dahle, H.K.</td>
<td>Streamline approach for a discrete fracture-matrix system</td>
</tr>
<tr>
<td>2009/3</td>
<td>Heimann, F.</td>
<td>An unfitted discontinuous Galerkin method for two-phase flow</td>
</tr>
</tbody>
</table>
2009/4  Hilfer, R. / Doster, F.: Percolation as a basic concept for macroscopic capillarity
2009/5  van Noorden, T.L. / Pop, I.S. / Ebigbo, A. / Helmig, R.: An effective model for biofilm growth in a thin strip
2009/6  Baber, K.: Modeling the transfer of therapeutic agents from the vascular space to the tissue compartment (a continuum approach)
2009/7  Faigle, B.: Two-phase flow modeling in porous media with kinetic interphase mass transfer processes in fractures
2009/8  Fritz, J. / Flemisch, B. / Helmig, R.: Multiphysics modeling of advection-dominated two-phase compositional flow in porous media
2009/9  Støverud, K.: Modeling convection-enhanced delivery into brain tissue using information from magnetic resonance imaging
2010/1  Rosenbrand, E.: Modelling biofilm distribution and its effect on two-phase flow in porous media
2010/2  Schöniger, A.: Parameter estimation by ensemble Kalman filters with transformed data
2011/1  Linders, B.: Experimental investigations on horizontal redistribution
2011/2  Rau, M.T.: Geostatistical analysis of three-dimensional hydraulic conductivity fields by means of maximum Gauss copula
2011/3  Kraus, D.: Two phase flow in homogeneous porous media - The role of dynamic capillary pressure in modeling gravity driven fingering
2011/4  Brugman, R.: Dimensionless analysis of convection enhanced drug delivery to brain tissues
2011/5  Sinsbeck, M.: Adaptive grid refinement for two-phase flow in porous media
2012/1  Köppl, T. / Wohlmuth, B. / Helmig, R.: Reduced one-dimensional modelling and numerical simulation for mass transport in fluids
2012/2  Kumar, K. / Pop, I.S. / Radu, F.A.: Convergence analysis for a conformal discretization of a model for precipitation and dissolution in porous media
2012/3  Hommel, J.: Modelling biofilm induced calcite precipitation and its effect on two phase flow in porous media
2012/4 Estrella, D.: Experimental and numerical approximation methods for zero-valent iron transport around injection wells

2012/5 Heimhuber, R.: Efficient history matching for reduced reservoir models with PCE-based bootstrap filters

2012/6 Kissling, F. / Karlsen, K.H.: On the singular limit of a two-phase flow equation with heterogeneities and dynamic capillary pressure

2012/7 Fritz, S.: Experimental investigations of water infiltration into unsaturated soil - Analysis of dynamic capillarity effects

2012/8 Strohmer, V.: Numerische Analysis von nahezu parallelen Strömungen in porösen Medien

2012/9 Kissling, F. / Rohde, C.: The computation of nonclassical shock waves in porous media with a heterogeneous multiscale method: The multidimensional case

2012/10 Fetzer, T.: Numerical analysis of the influence of turbulence on exchange processes between porous-medium and free flow

2012/11 Schröder, P.: A response surface bootstrap filter to calibrate CO₂ injection models


2013/2 Köppel, M.: Flow modelling of coupled fracture-matrix porous media systems with a two mesh concept

2013/3 van Helvoort, M.: Upscaling of processes involving rough boundaries

2013/4 Redeker, M. / Haasdonk, B.: A POD-EIM reduced two-scale model for crystal growth

2013/5 Vogler, D.: A comparison of different model reduction techniques for model calibration and risk assessment

2014/1 Song, N.: Investigation of a decoupling scheme for the modeling of reactive transport

2014/2 Aydogdu, A.B.: Phase field modelling of critical shear band evolution in granular media on the basis of a micropor medium theory

2014/3 Becker, B.: Investigation of error estimates for cell centered finite volume schemes: Analysis and improvement of grid adaptation strategies in DuMux

2014/4 Moghaddam, N.D.: Sorption of methane and ethane on Belgian black shale using a manometric setup

2014/5 Schwenck, N. / Flemisch, B. / Helmig, R. / Wohlmuth, B.: Dimensionally reduced flow models in fractured porous media: crossings and boundaries

2014/6 Redeker, M. / Pop, S. / Rohde, C.: Upscaling of a tri-phase phase-field model for precipitation in porous media


2014/9  Koch, T.: Coupling a vascular graph model and the surrounding tissue to simulate flow processes in vascular networks


2014/11  Seitz, G.: A conceptional approach to the effect of shear failure on the stress field in porous media

2014/12  Gläser, D.: Spatial model coupling for the simulation of CO2 injection scenarios in deep saline aquifers


2015/2  Bause, M. / Radu, F. A./ Köcher, U.: Error analysis for discretizations of parabolic problems using continuous finite elements in time and mixed finite elements in space

2015/3  van Duijn, C. J. / Cao, X. / Pop, I. S.: Two-phase flow in porous media: dynamic capillarity and heterogeneous media

2015/4  Pop, I. U. / Bogers, J. / Kumar, K.: Analysis and upscaling of a reactive transport model in fractured porous media involving a nonlinear transmission condition

2015/5  Jambhekar, V. A. / Mejri, E. / Schröder, N. / Helmig, R. / Shokri, N.: Kinetic approach to model reactive transport and mixed salt precipitation in a coupled free-flow-porous-media system


2015/9  Weishaupt, K.: Numerical modeling of steam chamber build-up guided by hot-water pre-injection


2015/11  Pluimers, S.: Hierarchical Fracture Modeling Approach

2015/12  Ostrowski, L.: Compressible Multicomponent Flow in a Porous Medium: Maxwell–Stefan Diffusion

2015/13  Cornelissen, P.: Coupled free-flow and porous media flow: a numerical and experimental investigation

2016/1  Ackermann, S.: Development and Evaluation of Iterative Solution Strategies for Coupled Stokes-Darcy Problems