Non-linearities and Upscaling in Porous Media

Spatial model coupling for the simulation of CO₂ injection scenarios in deep saline aquifers

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Abstract

In the realization of CO$_2$ storage projects, numerical simulations play an important role as they serve as a tool for the screening of potential storage sites, capacity estimations and risk assessments. However, the computational cost for such simulations is very high since both the multiphase flow processes and the mechanical response of the solid matrix have to be modeled. The resulting system of equations furthermore is strongly coupled and the spatial and temporal scales are very large. But, the importance of the different physical processes varies in space and time. For this reason a spatially coupled model has been developed, which solves for the fully coupled problem in regions adjacent to the injection well but neglects flow processes in the far field. Different concepts for the coupling have been implemented in the existing DuMu$^x$ framework and compared to a model of full complexity.


Las simulaciones numéricas de escenarios de inyección de CO$_2$ desempeñan un papel fundamental para la planificación de un proyecto semejante. A través de ellas, se puede evaluar la aptitud de una formación geológica, así como se pueden estimar los riesgos en relación con una inyección. La demanda computacional de la simulación de los procesos de flujo multifase y la reacción mecánica de la roca es muy alta, tanto por las ecuaciones fuertemente acopladas, como por las grandes escalas temporales y espaciales. Pero la importancia de los diferentes procesos varía en el espacio por cuya causa se puede aplicar el acoplamiento
de modelos de distinta complejidad en el espacio. Por esta razón fue realizado un modelo que resuelve el flujo multifase acoplado con la mecánica de la roca en las regiones adyacentes al pozo de la inyección, y que se reduce sólo a la mecánica de la roca en las zonas más alejadas. Diferentes conceptos del acoplamiento fueron implementados en el marco de DuMu$^x$ y comparados con un modelo que resuelve la entera complejidad del problema.
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List of symbols

Latin letters

- $B$: arbitrary body
- $B_0$: referential configuration of an arbitrary body $B$
- $g$: (scalar) gravitational acceleration [m/s$^2$]
- $\mathbf{g}$: vector of gravitational acceleration $(0, 0, -g)^T$ [m/s$^2$]
- $k_{r\alpha}$: relative permeability for phase $\alpha$
- $k_F$: hydraulic conductivity [m/s]
- $K$: intrinsic permeability Tensor [m$^2$]
- $p$: pressure [Pa]
- $p_\alpha$: pressure of phase $\alpha$ [Pa]
- $p_{\text{eff}}$: effective pressure [Pa]
- $p_{\text{el}}$: pseudo fluid pressure in the el-domain [Pa]
- $Q$: volumetric discharge of the well [m$^3$/s]
- $q$: source/sink term [kg/(s·m$^3$)]
- $q_\alpha$: source/sink term for phase $\alpha$ [kg/(s·m$^3$)]
- $R$: radius of influence [m]
- $S$: storage coefficient
- $S_\alpha$: saturation of phase $\alpha$
- $S_{r\alpha}$: residual saturation of phase $\alpha$
- $T$: transmissivity [m$^2$/s]
- $t$: time [s]
- $u$: solid displacement [m]
- $v$: velocity [m/s]
- $v_D$: Darcy velocity [m/s]
- $v_{D\alpha}$: Darcy velocity of phase $\alpha$ [m/s]
- $v_s$: displacement velocity of the solid matrix [m/s]
**Greek letters**

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<tr>
<th>Symbol</th>
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<tr>
<td>$\Gamma$</td>
<td>integration variable, represents the surface of a domain</td>
<td></td>
</tr>
<tr>
<td>$\Gamma_D$</td>
<td>part of the model domain consisting of the Dirichlet boundary conditions</td>
<td></td>
</tr>
<tr>
<td>$\Gamma_N$</td>
<td>part of the model domain consisting of the Neumann boundary conditions</td>
<td></td>
</tr>
<tr>
<td>$\mu_\alpha$</td>
<td>dynamic fluid viscosity of phase $\alpha$</td>
<td>kg/(s·m)</td>
</tr>
<tr>
<td>$\rho$</td>
<td>density</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$\rho_\alpha$</td>
<td>density of phase $\alpha$</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$\rho_b$</td>
<td>bulk density</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>stress tensor</td>
<td>N/m$^2$</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>flux of system property $\psi$ over the surface $\partial\Omega$</td>
<td></td>
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<tr>
<td>$\phi$</td>
<td>porosity</td>
<td></td>
</tr>
<tr>
<td>$\phi_{\text{eff}}$</td>
<td>effective porosity</td>
<td></td>
</tr>
<tr>
<td>$\Psi$</td>
<td>extensive system property</td>
<td></td>
</tr>
<tr>
<td>$\psi$</td>
<td>intensive system property</td>
<td></td>
</tr>
<tr>
<td>$\hat{\psi}$</td>
<td>production term of an intensive system property</td>
<td></td>
</tr>
<tr>
<td>$\Omega$</td>
<td>domain</td>
<td></td>
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**Mathematical notation**

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<tr>
<td>$\nabla$</td>
<td>gradient operator</td>
</tr>
<tr>
<td>$\text{div} (\cdot)$</td>
<td>divergence operator</td>
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**Subscripts**

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<td>$\alpha$</td>
<td>phase</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>CO$_2$ phase</td>
</tr>
<tr>
<td>eff</td>
<td>effective</td>
</tr>
<tr>
<td>n</td>
<td>non-wetting phase</td>
</tr>
<tr>
<td>s</td>
<td>solid matrix</td>
</tr>
<tr>
<td>w</td>
<td>wetting phase (brine)</td>
</tr>
<tr>
<td>0</td>
<td>at initial conditions</td>
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Chapter 1

Introduction

“Human Influence on the climate system is clear”. These words from the contribution of the working group 1 to the Fifth Assessment Report (AR5) of the Intergovernmental Panel on climate change (IPCC) (Stocker et al. (2013) [27]) should be capable of changing the minds of the last skeptic and disbelievers. Their statement is based on long and detailed observations, as well as sophisticated climate models that allow for a determination of the human contribution to the detected climate changes. The word climate is a measure for a number of meteorological parameters and their variations over a long period of time, and should not be confused with the actual weather. It is a result of the climate system with its components atmosphere, hydrosphere, cryosphere, lithosphere and biosphere. Thus, for the revelation of an actual climate change, investigations have to draw upon the observations of changes in certain indicators of each of these components and over large time scales. The IPCC (Stocker et al. (2013) [27]) offers a wide range of such data sets and corresponding interpretations.

Figure 1.1: Average combined land and ocean surface temperature anomaly 1850 - 2012 (figure taken from Stocker et al. (2013) [27])
The findings are alarming. As an example, figure 1.1 shows the evolution of the averaged combined land and ocean surface temperature. It can clearly be seen a trend towards higher temperatures and, even more worrying, the slope at which this is happening is increasing as well. The driving forces of climate change are substances and processes that affect the earth’s energy budget. Almost all the energy that affects the earth’s wheather originates from the sun in the form of radiant energy, which is partially absorbed and partially reflected by the planet and the atmosphere, i.e. the present substances. Long-wave radiation is furthermore radiated back into space.

For the purpose of estimating the impact of a substance on the radiation balance, Stocker et al. (2013) [27] use the parameter radiative forcing, which quantifies the difference in the energy fluxes relative to 1750, caused by a change in the concentration of the considered substance. Some substances may affect this balance more than others, however, it is stated that “the largest contribution to total radiative forcing is caused by the increase in the atmospheric concentration of CO$_2$ since 1750”. Expressed in numbers, of the estimated total anthropogenic radiative forcing of 2.29 W/m$^2$, 1.68 W/m$^2$ can be attributed to the anthropogenic emissions of CO$_2$ (from Stocker et al. (2103) [27]).

The correlating evolution of the atmospheric CO$_2$ concentrations (see figure 1.2) and the average temperature anomaly (figure 1.1) further substantiate this statement. The potential on mitigating the developments of a changing climate by lowering the emission is thus estimated to be very high. In Metz et al. (2007) [22] Carbon Capture and Storage (CCS) is therefore considered as a key technology in the battle against global warming. The general concept of CCS is outlined in the subsequent section, while in the sections 1.2 and 1.3 the motivation for this work and its structure are presented.

![Figure 1.2: Atmospheric CO$_2$ concentrations from Mauna Loa (red) and South Pole (black) since 1958 (figure taken from Stocker et al. (2103) [27])](image-url)
1.1 Carbon capture and storage (CCS)

Carbon Capture and Storage, or geological sequestration, describes technologies in which CO\textsubscript{2} that would otherwise be emitted into the atmosphere, is captured, compressed and transported to and injected into a suitable geological formation. The technology can be directly applied to large stationary sources and hence offers a big potential. With respect to geological formations that are suitable for such an injection, there are several options.

Depleted oil or gas reservoirs have proven in the past their capability of safely storing and trapping a fluid. Furthermore, CO\textsubscript{2} enhanced oil recovery technologies exist, where CO\textsubscript{2} is injected for the exploitation of oil that would otherwise be trapped. The injection of CO\textsubscript{2} leads to an increased reservoir pressure and reduces the viscosity of the oil, which makes it exploitable. Note that in this technology the oil is piped in a cycle for what reason it can not be stored large quantities. The sequestration in unmineable coal beds is also possible and economically attractive as methane, absorbed to the present coal, can be extracted during this process.

Another group of geological formations are deep saline aquifers. These formations are very common worldwide and thus offer a great storage potential. They are characterized by holding a saline pore fluid that is of no special use for humanity, so a direct conflict with other applications will not be faced. An overview over the different storage possibilities is given in figure 1.3.

Figure 1.3: Possible geological formations for CO\textsubscript{2} injection (Courtesy CO2CRC)
1.2 Motivation for this work

However, an injection always involves some risks. Suitable deep saline aquifers exhibit a low permeable layer on top, which prevents the CO$_2$ from migrating upwards. But the existence of faults or cracks can lead to leakage and an upwards flow of CO$_2$ into shallower formations. This could lead to potential conflicts with other applications, as for example groundwater production or geothermal applications. The stress imposed on the reservoir by the injection can cause such cracks or faults to open up or to be created. These risks have to be determined in advance, where numerical simulations come into play. The results obtained by numerical simulations give an idea of how the CO$_2$ will spread and behave in the aquifer, of how the pressure will evolve and of the mechanical reaction of the formation’s rock on the stress resulting from the injection.

1.2 Motivation for this work

Unfortunately, the computational cost for the simulation of CO$_2$ injection scenarios is very high. This is caused on one hand by the large spatial and temporal scales that have to be considered. On the other hand, the set of equations that describe the flow of the two phases within the pore space including the mechanical response of the rock is strongly coupled and non-linear. However, since the physical processes involved in such an injection vary in space and time, it thus arises the idea of neglecting certain processes in certain parts of the domain depending on the time spans. It thus are solved models of different complexity in different parts of a considered domain, which is why this approach is called spatial model coupling. The actual motivation for the application of such a coupling to the regarded problem will be given in section 4.1. In this work, spatially coupled models have been developed and tested by drawing a comparison to a model of full complexity.

1.3 Structure of the thesis

In subsequent chapter, the physical processes involved in injection scenarios of CO$_2$ into deep saline aquifers are described in a phenomenological way. Then, the quantities that appear in the description of these processes are presented and explained, and it is outlined a general way of deriving the equations that allow for the description of the involved physics. In chapter 3, the mathematical foundation which is used for the solution of these equations is introduced, as well as further mathematical concepts that form part of this work. Chapter 4 presents the actual problem, i.e. the descriptive equations and their derivation. Furthermore, it is explained the way the spatial coupling is realized and the different approaches for the treatment of the appearing interface. In chapter 5, the results are presented before they are further summarized, discussed and an outlook on future work is given in chapter 5.
Chapter 2

Fundamentals

2.1 CCS - the physics

A large number of physical processes is involved in CO$_2$ injection scenarios. However, they strongly vary in space and time, occur on different time scales and/or consecutively. The early times after injection start are characterized by a large pressure buildup in the regions close to the injection well and initially very steep pressure gradients. The mutual solubility of CO$_2$ and brine is relatively low, thus the system at this point is an advection dominated multiphase flow system provoked by these gradients, as well as buoyant, viscous and capillary forces. Buoyancy effects originate from the density difference between the two phases and lead to an upward migration of the CO$_2$ until it eventually reaches the sealing caprock. The CO$_2$ hence spreads in the form of a plume.

The pressure signal induced by the injection has significant effects on a much larger scale than where CO$_2$ is actually observable, potentially causing the migration of deep brines into shallower formations, which in turn could lead to conflicts with groundwater production or other applications. Besides the hydrodynamic processes, geomechanical phenomena are important since the large pressure buildup leads to a reduction of the compressive stresses within the solid matrix, which are a result from the load of the overburden. As a consequence of this, deformations of the solid occur which in turn lead to an increased porosity and permeability\footnote{Note that the in this section mentioned physical quantities and parameters will be explained in the subsequent sections}. These changes in the hydraulic properties of the aquifer on the other hand allow the initially steep pressure gradients to smoothen out faster, which again affects the mechanical response of the rock. The physical processes are thus strongly coupled. The rock’s mechanical reaction on the injection is furthermore very important for risk assessment studies, as a widening or opening up of cracks can be induced, potentially establishing migration paths for the CO$_2$ into shallower horizons.

On top of that, the temperature difference between the injected CO$_2$ and the reservoir causes temperature changes and can lead to a change in the properties of both rock and
With time phase transfer processes become more important. The injected CO\textsubscript{2} is generally undersaturated with respect to water, which leads to a dissolution of water from the residual brine close to the injection well. It thus results a one phase flow system in these regions and in addition to that, caused by the precipitation of the originally dissolved salt in the residual brine, a change of the hydraulic parameters is likely to occur. As mentioned before, the CO\textsubscript{2} migrates upwards forming the shape of a plume. This plume shaped propagation results in a larger interphase between the two phases and to an increased importance of phase transfer processes. At great distances to the injection well, and especially when the injection has been ceased, the CO\textsubscript{2} ends up sandwiched between the caprock and the brine and slowly dissolves in it. Unlike it is the fact for most gases, dissolved CO\textsubscript{2} leads to an increase in the brine’s density, which in turn results in an unstable layering within the water phase and leads to a downward migration and fingering of the CO\textsubscript{2}-rich brine. The surface area between the phases is thus increased and the dissolution enhanced. However, the time scales for these processes are substantially larger than for the primarily mentioned phenomena. On even larger time scales, geochemical processes can become important and involve mineral precipitation of the CO\textsubscript{2}. This can again affect the aquifer properties and can lead to a sealing of prevailing or the creation of new flow paths.

2.2 The porous medium

“Initially, we may attempt to describe a porous medium as a solid with holes”\textsuperscript{2} This rather rough statement in Bear (1972) \cite{Bear1972} is followed by a long and detailed definition of the porous medium. The lecture of this passage makes one realize that defining such a medium accurately is not as easy as expected, however, it is now tried to point out some characteristics of porous media by citing a few of his statements:

\begin{enumerate}
\item A porous medium is “a portion of space occupied by heterogeneous or multiphase matter”
\item “At least one of the phases comprising this matter is not solid”
\item “That space within the porous medium domain that is not part of the solid matrix is referred to as void space (or pore space)”
\end{enumerate}

\textsuperscript{2}Bear (1972) \cite{Bear1972}, p.14


(4) “At least some of the pores comprising the pore space should be interconnected”

(5) “Solid must be present inside each representative elementary volume”

The first statement clarifies that when dealing with porous media, one has to deal with multiphase systems. Furthermore, a solid matrix is present (2), in which flow can occur through designated flow paths (4) and the phases that are not part of the solid phase occupy the pore space (3). After defining the porous medium it now arises the question of how to describe its physical behaviour. Statement (5) brings up the concept of a representative elementary volume. An REV is a control volume chosen large enough so that a statistical averaging process can be derived and a physical quantity can be expressed by its average value inside the control volume. For the exact geometry, i.e. the phase distribution and the flow paths of the porous medium, that concept equals a smearing over the control volume, neglecting the exact geometry and considering only the amount of a phase within the control volume. The multiphase system is thus treated like a mixture. An illustration of the smearing is shown in figure 2.1.

Figure 2.1: Illustration of the smearing of a porous medium

As indicated in the above figure, in reality it is dealt with a multiphase system, with its constituents occupying designated parts of it due to their physical properties. For its description as a smeared system, a mixture, Truesdell’s three metaphysical principles are generally taken as a theoretical paradigm (Truesdell (1984) [29]):

(1) All properties of the mixture must be mathematical consequences of the properties of the constituents

(2) So as to describe the motion of a constituent, we may in imagination isolate it from the rest of the mixture, provided we allow properly for the actions of the other constituents upon it
The motion of the mixture is governed by the same equations as is a single body.

A direct result of (2) is that we consider the mixture to comprise of superimposed constituents that interact mutually. There is thus no more spatial separation of the constituents regarded inside the control volume. For the description of the different constituents or phases $\alpha$ inside the mixture as promoted by (2), it is accounted for their particular amount through their volume fraction:

$$n_\alpha = \frac{V_\alpha}{V_{CV}}. \quad (2.1)$$

The new introduced quantity is a direct result of the upscaling and neglecting of the exact geometry. When dealing with multiphase flow inside the pore space of a solid matrix, the processes are mostly described within this space. For this purpose the porosity is introduced, allowing for a more convenient description.

### 2.2.1 Porosity

The porosity is defined as the relation between the pore space and the entire space of the control volume:

$$\phi = \frac{V_{\text{pore}}}{V_{CV}} = 1 - n_{\text{solid}}. \quad (2.2)$$

### 2.2.2 Saturation

The above introduced porosity now allows for the description of only the pore space, which is very convenient for the modeling of flow processes within a rigid porous matrix. However, when the motion of more than one phase is sought to describe, the saturations have to be introduced to account only for a particular phase $\alpha$. The definition of the saturation is analogous to the one of the volume fraction (2.1), but now relating the volume of phase $\alpha$ to the pore volume:

$$S_\alpha = \frac{V_\alpha}{V_{\text{pore}}} \frac{2.1}{2.2} \frac{n_\alpha}{\phi}. \quad (2.3)$$

A natural result of the definition of the saturation is that the sum of all saturations must add up to 1:

$$\sum_\alpha S_\alpha = 1. \quad (2.4)$$
2.2 The porous medium

With the new quantities at hand, it can now be described multiphase flow in porous media without considering the exact geometry of the original multiphase system. But in addition to that, physical processes and quantities on the pore scale have to be abstracted and transferred to the upscaled description, since upscaling generally involves a loss of information on the physics that occur on a smaller scale. These have to be included on the coarse scale by adequate relations or parameters that depend on its quantities. In the following the quantities and relations appearing in the models of this work are outlined.

2.2.3 Intrinsic permeability

The size, shape and connectivity of the pores within the REV determine the resistance of the porous medium on the flow of the fluid phases. Since the exact geometry of the pores is no longer resolved, this effect has to be included in the description on the REV scale by the introduction of a new quantity, the intrinsic permeability $K$. It appears in Darcy’s Law (see section 2.4), which is mostly used for porous medium applications.

$K$ is defined as a tensor, since the pore widening and connectivity of the pores generally varies for different space directions. Sedimentary rocks in particular show such an anisotropy because of their natural layered structure, leading to higher permeabilities in horizontal than in vertical directions. In general, the porosity and permeability are two independent quantities, however, a higher porosity usually results in a higher permeability. But, a larger influence on the permeability is imposed by the rock type, which determines e.g. the connectivity of the pores. For example, sandstones can exhibit permeabilities in the range of several orders of magnitude higher than shale, even though shales potentially show larger porosities (Fjaer et al. (2008) [15]).

2.2.4 Relative permeability

The above mentioned resistance, included in the intrinsic permeability, only accounts for the resistance the porous medium bears on the flow within its pore space. In multiphase systems the pore space is shared by more than one phase and thus less pore space is available. Furthermore, depending on the wettability of a phase, it occupies certain parts of the porous medium (see figure 2.1). The wetting fluid is dragged into the small pores and dead ends, as it wants to cover more of the pore surface, whereas the non-wetting fluid essentially is found in the bigger pores. The presence of another pore fluid thus imposes further resistance on the flow of the other fluid phases, which is not included in the intrinsic permeability. It thus has to be introduced a relative permeability $k_r$, which is multiplied with the intrinsic permeability and which describes this mentioned resistance to flow. It furthermore has to be expressed by the quantities available on the REV scale. Brooks and Corey (1964) [8] came up with an expression for $k_r$ dependent on the saturation, which for a two phase system consisting of a wetting phase $w$ and a non-wetting phase $n$ reads as follows:
2.2 The porous medium

\[ k_{rw} = S_e^{2+\lambda_{BC}} \quad \text{(2.5)} \]

\[ k_{rn} = (1 - S_e)^2 \left( 1 - S_e^{2+\lambda_{BC}} \right) \quad \text{(2.6)} \]

The fitting parameter \( \lambda_{BC} \) reflects the grain size distribution of the porous medium. For homogeneous media, i.e. a rather narrow grain size distribution, \( \lambda_{BC} \) becomes large. In contrast, heterogeneous media are characterized by relatively small values for \( \lambda_{BC} \) (Ochs (2006) [25]) and thus show higher resistance to flow for the wetting phase. The effective saturation

\[ S_e = \frac{S_w - S_{rw}}{1 - S_{rw}} \quad \text{(2.7)} \]

is a function of the wetting phase saturation \( S_w \) and its residual saturation \( S_{rw} \). The residual saturation represents the amount of wetting phase, that cannot be displaced by the non-wetting phase and that is therefore trapped in the porous medium. It thus affects the extent of the CO\(_2\) plume since for large residual saturations less pore space is available and a larger volume of the aquifer has to be occupied in order to store the injected CO\(_2\).

### 2.2.5 Capillary pressure

As already mentioned, the wetting fluid tends to occupy the small pores and dead ends, driven by the adhesive force at the interphase with the solid. As a consequence of that, a pressure difference at the interphase between the wetting and the non-wetting phase is established, which is called the capillary pressure:

\[ p_c = p_n - p_w. \quad \text{(2.8)} \]

The description of the porous medium happens on the REV scale, thus it again has to be found a description of the capillary pressure as a function of the REV-scale quantities. The Brooks and Corey (1964) [8] relation

\[ p_c = p_d S_e^{-1/\lambda_{BC}} \quad \text{(2.9)} \]

is used in this work, where \( S_e \) and \( \lambda_{BC} \) are the above introduced parameters. \( p_d \) is the entry pressure that has to be overcome by the non-wetting phase in order to enter a porous medium fully saturated with the wetting phase.
2.3 Conservation equations

The modeling of fluid flow generally requires the formulation of the balance equations for the system’s quantities mass, momentum and energy. In addition to that, constitutive equations have to be formulated for the closure of the system, which have to fulfill the entropy inequality in order to maintain physical significance. In the following a general approach for the formulation of a balance equation for an extensive system property \( \Psi \) and the derivation of the mass balance as well as the momentum balance equation is presented. Note that the shown derivations are performed for a single phase system.

2.3.1 General approach

Consider an arbitrary body \( B \) with domain \( \Omega \), surface \( \Gamma_\Omega \), the respective normal vector \( n \) and with \( d\Gamma_\Omega \) being the normal vector to a small patch on the surface \( \Gamma_\Omega \) (see figure 2.2). The overall amount of the property \( \Psi \) in the domain \( \Omega \) then is

\[
\Psi = \int_\Omega \rho \psi \, d\Omega, \tag{2.10}
\]

with \( \psi \) being the corresponding intensive property \( \psi = \frac{d\Psi}{dm} \). A general master balance law for the conservation of an intensive quantity can be formulated as follows:

\[
\frac{d}{dt} \int_\Omega \rho \psi \, d\Omega = \int_{\Gamma_\Omega} \varphi \cdot n \, d\Gamma_\Omega + \int_\Omega q \, d\Omega + \int_\Omega \hat{\psi} \, d\Omega. \tag{2.11}
\]

Here, \( \varphi \) is the flux of the quantity over the surface \( \Gamma_\Omega \), \( q \) denotes sources or sinks and \( \hat{\psi} \) is a production term within the domain \( \Omega \). Note that all of the presented variables can be functions of both space and time. Metaphorically speaking, equation (2.11) equalizes the temporal change of \( \Psi \) to the sum of the processes that come along with a change of this property.
In general the body B is deformable and its movement has to be considered. The expansion of the left hand side of the equation and using the notation of the material time derivative \( \frac{dx}{dt} = \dot{x} \) thus leads to

\[
\frac{d}{dt} \int_{\Omega} \rho \psi \, d\Omega = \int_{\Omega} \left[ (\rho \dot{\psi}) + \rho \psi \text{div}(\mathbf{v}) \right] d\Omega, \tag{2.12}
\]

where the identity \( d\Omega = \text{div}(\mathbf{v}) d\Omega \) has been used (please see details in Appendix A). Applying the material time derivative

\[
(\rho \dot{\psi}) = \frac{\partial (\rho \psi)}{\partial t} + \mathbf{v} \cdot \nabla (\rho \psi), \tag{2.13}
\]

the product rule of differentiation

\[
\text{div}(\rho \psi \mathbf{v}) = \mathbf{v} \cdot \nabla (\rho \psi) + \rho \psi \text{div}(\mathbf{v}), \tag{2.14}
\]

and the Green-Gaussian integral rule

\[
\int_{\Omega} \text{div}(\rho \psi \mathbf{v}) \, d\Omega = \oint_{\Gamma_B} \rho \psi (\mathbf{v} \cdot \mathbf{n}) \, d\Gamma \tag{2.15}
\]
on the left side of equation (2.12) leads to

\[
\frac{d}{dt} \int_{\Omega} \rho \psi \, d\Omega = \int_{\Omega} \frac{\partial (\rho \psi)}{\partial t} \, d\Omega + \oint_{\Gamma_B} \rho \psi (\mathbf{v} \cdot \mathbf{n}) d\Gamma. \tag{2.16}
\]

This equation is known as the Reynolds transport theorem and represents the relationship between the lagrangian and the eulerian description of a time-dependent control volume. The second term on the right side can be seen as the flux over the surface related to flow processes. Now the Green-Gaussian integral rule is again applied on equation (2.16) and on the flux term on the right side of equation (2.11). Additionally, the localization theorem \( d\Omega \rightarrow 0 \) is used under the assumption that all integrands are continuous:

\[
\frac{\partial (\rho \psi)}{\partial t} + \text{div}(\rho \psi \mathbf{v}) = \text{div}(\varphi) + q + \hat{\psi}. \tag{2.17}
\]

Based on this equation, appropriate balances for the system properties can be obtained by inserting the adequate intensive quantities and providing suitable models for the mathematical description of the flux, the source and the production term. Note that in single phase systems the production term vanishes for the mass, momentum and energy balance and only forms a part in the entropy inequality equation. In multiphase systems, this term generally does not cancel out, but is used to account for the exchange of the property between the different phases.
2.3 Conservation equations

2.3.2 Mass balance equation

The conservation of mass is a fundamental axiom:
\[
\frac{d}{dt} M = \frac{d}{dt} \int_{\Omega} \rho \psi \, d\Omega = 0. \tag{2.18}
\]

The respective differential equation can be derived by inserting \( \psi = 1 \) in equation (2.17):
\[
\frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{v}) = q. \tag{2.19}
\]

2.3.3 Momentum balance equation

Newton’s second law states the relationship between an object’s mass \( m \), it’s acceleration \( a \) and the sum of forces \( \mathbf{F} \) acting on it:
\[
\mathbf{F} = ma. \tag{2.20}
\]

As a consequence, for the momentum
\[
\mathbf{P} = m\mathbf{v} = \int_{\Omega} \rho \mathbf{v} \, d\Omega \tag{2.21}
\]
the following conservation equation holds:
\[
\frac{d}{dt} \mathbf{P} = \frac{d}{dt} \int_{\Omega} \rho \mathbf{v} \, d\Omega = \mathbf{F}. \tag{2.22}
\]

Let now be gravity the source of momentum and \( \mathbf{t} \) a force acting on the surface of the body (see figure 2.3 in section 2.5). Applying Cauchy’s theorem \( \mathbf{t} = \mathbf{T} \mathbf{n} \) allows for the derivation of the respective differential equation by inserting \( \psi = \mathbf{v} \) in equation (2.17). For a single phasic material the production term \( \dot{\psi} \) is set to zero:
\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \text{div}(\rho \mathbf{v} \otimes \mathbf{v}) = \text{div}(\mathbf{T}) + \rho \mathbf{g}. \tag{2.23}
\]

After the expansion of the left side of eq. (2.23) to
\[
\rho \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \frac{\partial \rho}{\partial t} + \rho \mathbf{v}^{T} \nabla \mathbf{v} + \mathbf{v} \text{div}(\rho \mathbf{v}), \tag{2.24}
\]
the mass balance equation (multiplied by the velocity \( \mathbf{v} \)) can be identified combining the
second and the fourth term and can thus be canceled out in the case of \( q = 0 \). Also, the first and third term add up to the material time derivative \( \rho \dot{\mathbf{v}} \). It results the momentum balance equation for a single phasic material:

\[
\rho \dot{\mathbf{v}} = \text{div}(\mathbf{T}) + \rho \mathbf{g}.
\] (2.25)

### 2.4 Darcy’s Law

Darcy’s law was originally found by the French engineer Henry Darcy (* 06/10/1803 in Dijon, France; † 01/03/1858) as a result of experiments he undertook on the flow of water through columns of sand (Darcy (1856) [13]). However, a derivation can also be performed based on the momentum balance equation (2.25) for a single fluid phase \( F \) in the pore space of a solid matrix \( s \):

\[
\rho_F \dot{\mathbf{v}}_F = \text{div}(\mathbf{T}_F) + \phi \rho_F \mathbf{g} + \hat{p}_F. \tag{2.26}
\]

The momentum production term \( \hat{p}_F \) represents the interaction, i.e. the exchange of momentum of the pore fluid with the solid matrix. For the further derivation, the following assumptions are made:

- **(A1)** Creeping flow regime \( \text{Re} \ll 1 \)
  \[ \rightarrow \rho_F \dot{\mathbf{v}}_F = 0 \]

- **(A2)** Solid and fluid are immiscible
  \[ \rightarrow \hat{p}_F = 0 \]

- **(A3)** Incompressible fluid and solid matrix
  \[ \rightarrow \rho_F = \text{const.}, \rho_s = \text{const.} \]

- **(A4)** Rigid solid matrix
  \[ \rightarrow \mathbf{v}_s = 0 \]

\[ \hat{p}_F \] would have appeared in the momentum balance equation as a fragment of the mass balance equation, which has been canceled out in the derivation process for a single phasic material. However, in the case of immiscibility \( \hat{p}_F = 0 \)
The following relation holds for the stress tensor $T_F$ of a general compressible fluid:

$$T_F = -\phi p I + 2\mu_F D_F + \lambda_F (D_F : I) I = -\phi p I + T_E^F,$$  \hspace{1cm} (2.27)

where $D_F = \nabla v$ is the velocity gradient, $\mu_F$ denotes the dynamic viscosity and $\lambda_F$ the volumetrical viscosity. Dimensional analyses show, that the extra stress $T_E^F$, induced by the viscosity, is very small in comparison to the momentum production term (or exchange term) $\hat{p}_F^E$ for small characteristic lengths and is therefore neglected in the following. The latter is defined as:

$$\hat{p}_F = p \nabla \phi + \hat{p}_E^F = p \nabla \phi - \phi^2 \mu_F K^{-1} w_F.$$  \hspace{1cm} (2.28)

Here, $p$ indicates the effective pore pressure and $\hat{p}_E^F$ again is an extra quantity induced by the viscosity. Furthermore, $w_F = v_F - v_s$ is the seepage velocity and $K$ the intrinsic permeability tensor. After insertion of these constitutive equations and neglecting the extra stress $T_E^F$, one obtains:

$$\text{div}(-\phi p I) + \phi \rho_F g + p \nabla \phi - \phi^2 \mu_F K^{-1} v_F = 0$$  \hspace{1cm} (2.29)

and after expansion of the divergence term:

$$-p \nabla \phi - \phi \nabla p + \phi \rho_F g + p \nabla \phi - \phi^2 \mu_F K^{-1} v_F = 0.$$  \hspace{1cm} (2.30)

The equation can now be rearranged for the determination of the Darcy velocity $v_D = \phi v_F$:

$$\phi v_F = v_D = -\frac{K}{\mu_F} (\nabla p - \rho_F g).$$  \hspace{1cm} (2.31)

Further using the relationship between the hydraulic conductivity and the intrinsic permeability $K = K_h \frac{\mu_F}{\rho_F |g|}$, equation (2.31) can be rewritten to

$$v_D = K_h (\nabla \frac{p}{\rho_F |g|} - e_3) = -K_h \nabla h,$$  \hspace{1cm} (2.32)

where the definition of the piezometric head

$$h = \frac{p}{\rho_F |g|} + x_3$$  \hspace{1cm} (2.33)

has been used. In multiphase systems, Darcy's law (2.31) has to be extended by the relative permeability (see section 2.2), in order to describe the mutual interaction of the
different phases on their flow behaviour. The standard multiphase Darcy’s approach reads:

\[ v_{D\alpha} = -\frac{k_{r\alpha}}{\mu_{\alpha}} K (\nabla p_{\alpha} - \rho_{\alpha} \mathbf{g}). \] (2.34)

Note that this last equation can also be derived formally, however, at this point it is referred to the literature. It is again pointed out, that because of the assumptions made during the derivation process above, Darcy’s Law is only valid for slow and laminar flow. It is established that for Reynolds numbers less than one equation 2.31 or 2.34 hold (assumption (A1)), which is the case for most porous medium applications.

2.5 Rock mechanics

In the above sections it has been looked at the fluid flow inside the pore space of the porous medium, i.e. the solid skeleton. However, one major focus of the models in this work is on the deformations of the solid skeleton due to the injection of \( \text{CO}_2 \). In order to describe mechanical deformations of a solid body, its momentum balance equation has to be solved and, for the closure of the equation system, a particular material law has to be formulated. This individual material law describes the reaction of a solid on external loads. If geological formations are to be modeled, one has to keep in mind that the mechanical properties of rock on one hand strongly depend on the rock type, i.e. the general way it was formed, but also on the particular history of a formation.

Rock types

There are three types of rocks, which are distinguished based on their genesis. Igneous rocks are formed by solidified lava that was blown out during volcanic eruptions. An example for such formations is the ocean bed of the atlantic ocean, formed by the basic lava rupturing out of the mid-ocean ridge. Sedimentary rocks are the result of chemical and mechanical erosion of other rock types. The eroded material accumulates in sedimentary basins and thus sedimentary rocks are usually found near the earth’s surface. With more material being deposited on top of the sediments, the grains get more and more compacted and with time a cementation of the material takes place. The resulting mechanical properties of the rock depend on the type of material, as well as on the grain size, shape and sorting and can vary substantially. The third type is metamorphic rock, which forms out of the previously described rock types under the influence of stress and heat, e.g. in subduction zones.

Igneous and metamorphic rocks are typically not suitable for \( \text{CO}_2 \) storage, since they are often too fractured and situated in great depths (Darcis (2013) [12]). This leaves sedimentary rocks as the type of interest for this work. As mentioned before, the mechanical properties depend on the type and amount of cementing material. On top of that, on larger scales the formation might exhibit faults and cracks, which have an influence on the properties depending on the size of these faults with respect to the considered mass of rock.
and the rock’s frictional resistance. If sliding can be excluded though, the regarded body of rock can be considered as a continuum.

**Continuum mechanical description**

Continuum mechanics aim for the description of what is going on inside a body while not resolving the motions and forces of atoms or other sub-scale constituents. The continuum is seen as an idealized space filled with continuous matter and continuous properties. The scale of the regarded body thus has to be large enough to allow for the neglecting of property variations that appear on the molecular scale, e.g. density fluctuations.

**The material law**

In equation (2.25) the stress tensor $T$ appears, for which was given an expression for a general compressible fluid in section 2.4. Analogously to that it has to be found an expression with respect to the mechanical behaviour of the solid, i.e. a material law. In this work it is applied a linear elastic material law in the context of the *small deformation theory*. The quantities emerging in it are further explained in the sequel.

**2.5.1 Basic kinematic considerations**

Consider a random body. The material points of this body in its referential configuration are denoted by the coordinates $X$. The body now undergoes translations and rotations under the influence of an external force $t$ and body forces $b$ (e.g. gravity), transforming it into its actual configuration. The material points of the actual configuration are characterized by the coordinates $x$ and the displacement that one material point has experienced is denoted by $u$ (see fig. 2.3).

![Figure 2.3: Arbitrary Motion of an exemplary body and forces acting on it](image)

4The author has in mind that strictly speaking the density does not exist on the molecular scale, it is instead a quantity that appears on the continuum scale. Nevertheless, for a description of a solid on the continuum scale, the regarded domain has to be large enough to exclude density variations.
2.5 Rock mechanics

Strain

During the transformation of the body, the material points very likely change their relative position with respect to each other. The body is thus called to be strained. While the displacements $u$ give a measure of absolute position changes, the strain measures relative changes in the displacement field, i.e. its spatial gradients. Consider now the displacements $u$ at the position $x$ very close to the position $x_0$. $u$ can then be expanded in a Taylor series ignoring higher order terms, i.e. the products of the partial derivatives. The assumption that these products are negligible small is the basis of the above mentioned small strain theory:

$$u(x) = u(x_0) + \frac{\partial u}{\partial x} d = u(x_0) + H \frac{\partial u}{\partial x} d.$$  \hspace{1cm} (2.35)

Here, $d = x - x_0$ and

$$H = \nabla u = \begin{pmatrix} \frac{\partial u_x}{\partial x} & \frac{\partial u_x}{\partial y} & \frac{\partial u_x}{\partial z} \\ \frac{\partial u_y}{\partial x} & \frac{\partial u_y}{\partial y} & \frac{\partial u_y}{\partial z} \\ \frac{\partial u_z}{\partial x} & \frac{\partial u_z}{\partial y} & \frac{\partial u_z}{\partial z} \end{pmatrix}.$$  \hspace{1cm} (2.36)

is the displacement gradient tensor. $H$ can further be split into the symmetric strain tensor and the antisymmetric rotation tensor:

$$H = \frac{1}{2} (\nabla u + \nabla^T u) + \frac{1}{2} (\nabla u - \nabla^T u) := \epsilon + \Omega.$$  \hspace{1cm} (2.37)

The rotation tensor causes rigid rotation without a relative volume decrease, or dilatation. The strain tensor causes strain through its off-diagonal components and the dilatation is given by

$$\Delta = \text{tr} [\epsilon] = \text{div}(u) = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}.$$  \hspace{1cm} (2.38)

Stress

The normal stress $\sigma$ is defined as the ratio between a normal force acting on a plane and the plane’s surface:

$$\sigma = \frac{F_n}{A}.$$  \hspace{1cm} (2.39)

Corresponding to that it is defined the shear stress which is caused by forces acting tangential to the regarded plane:

$$\tau = \frac{F_t}{A}.$$  \hspace{1cm} (2.40)
2.5 Rock mechanics

In three dimensions, the stress tensor $\tau$ has nine independent entries. However, since the solid is in static equilibrium, there can be no net rotation from the shear stresses. As a consequence, the stress tensor has to be symmetric (now denoted with $\sigma$). This also results formally from the balance of angular momentum for the assumption of small strains (see section 4.2):

$$\sigma = \begin{pmatrix}
\sigma_x & \tau_{xy} & \tau_{xz} \\
\vdots & \sigma_y & \tau_{yz} \\
\vdots & \vdots & \sigma_z
\end{pmatrix}. \quad (2.41)$$

2.5.2 The linear stress-strain relationship

Stress and strain, and essentially the stress and the displacements, are now linked in a constitutive relationship. This so called material law is needed for the closure of the equation system (see section 4.2). Since it is asked to be linear and both strain and stress have nine entries, in general a fourth order tensor is required to link them:

$$\tau = C \epsilon, \quad (2.42)$$

or in index notation using the summation convention:

$$\tau_{ij} = c_{ijkl} \epsilon_{kl} = \sum_{k=1}^{3} \sum_{l=1}^{3} c_{ijkl} \epsilon_{kl}. \quad (2.43)$$

$C$ is also called the elastic tensor. The 81 independent entries of $C$ can be reduced to 21 because of the symmetry of the stress and strain tensor (see above). These components are necessary to specify the linear elastic behaviour of a general anisotropic solid. In this work it is further assumed isotropy (discussion see following section), which reduces the number of parameters to two:

$$c_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{il} \delta_{jk} + \delta_{ik} \delta_{jl}), \quad (2.44)$$

with $\lambda$ and $\mu$ being the two Lamé parameters. Inserting the above relation into the linear relation (2.43) and using $\epsilon_{ij} = \epsilon_{ji}$ leads to the linear elastic material law for an isotropic solid:

$$\sigma = \lambda \mathrm{tr} [\epsilon] I + 2\mu \epsilon. \quad (2.45)$$
2.5 Rock mechanics

The parameter $\mu$ is the shear modulus and describes the ratio of shear stress and corresponding shear strain

$$\mu = 0.5 \left( \frac{\tau_{xz}}{\epsilon_{xz}} \right),$$

(2.46)

whereas for Lamé's constant $\lambda$ there is no physical interpretation. Furthermore, the mechanical parameters of rock are typically specified in terms of Young's modulus $E$, defined as the uniaxial ratio of stress and strain

$$E = \frac{\sigma_z}{\epsilon_z},$$

(2.47)

and Poisson’s ratio $\nu$:

$$\nu = -\frac{\epsilon_x}{\epsilon_z}.\quad (2.48)$$

$\nu$ sets into relation the longitudinal strain $\epsilon_x$ to the transverse strain $\epsilon_z$, both caused by a compression or expansion in longitudinal direction.

However, the two Lamé parameters can then be calculated from $E$ and $\nu$ using the following relations:

$$\lambda = \frac{E\nu}{(1 + \nu)(1 - 2\nu)}\quad (2.49)$$

$$\mu = \frac{E}{2 + 2\nu}.\quad (2.50)$$

2.5.3 Poroelasticity

The above introduced fundamentals of continuum mechanics were derived for a single continuum. In order to describe the mechanics of a fluid-saturated porous medium, the concepts have to be extended in order to take into account the influence of the pore fluids on the mechanical behaviour of the solid matrix. External loads acting on the medium will partially be supported by the pore fluids and thus stresses in the porous medium result smaller. In the case of an elastic solid, as it is in the models of this work, the medium is called poroelastic and for its description one can consult the theory of poroelasticity.

The theory of poroelasticity has been developed by the Belgian-American physicist Maurice Anthony Biot (* 05/25/1905 in Antwerpen, Belgium; † 09/12/1985 in New York) in a series of papers. In 1941 [7] he came up with a formulation of the effective stress law:

$$\sigma' = \sigma - \alpha p l.$$

(2.51)
In this equation $\sigma'$ denotes the effective stress and $\alpha$ is the biot parameter. The concept of effective stresses had been introduced a few years earlier by Karl von Terzaghi, however, Biot’s contribution was the parameter $\alpha$ which is a function of the bulk modulus of the porous medium $K_b$ and of the solid grains $K_g$:

$$\alpha = 1 - \frac{K_b}{K_g}. \quad (2.52)$$

The bulk modulus furthermore describes the resistance to hydrostatic compression and is defined as the ratio between the average normal stress $\sigma_p$ and the volume dilatation $\Delta = \text{tr} [\epsilon]$ (see equation (2.38)):

$$K = \frac{\sigma_p}{\text{tr} [\epsilon]}. \quad (2.53)$$

Biot’s parameter thus approaches one for highly porous media and becomes zero if the rock is poorly permeable, i.e. does not exhibit many interconnected pores. The linear elastic material law presented in the last section can now be extended by the fluid pressure and a description in effective stresses. However, in this work it is considered multiphase flow and therefore the pressure has to be replaced by the effective pressure $p_{eff}$:

$$\sigma' = \lambda \text{tr} [\epsilon] I + 2\mu \epsilon - p_{eff} I, \quad (2.54)$$

with

$$p_{eff} = S_w p_w + S_n p_n. \quad (2.55)$$

### 2.5.4 Effective porosity

The displacements of the solid matrix further affect the properties of the porous medium, more precisely it will lead to a change in porosity. This change in porosity on the other hand influences the fluid flow, which is a reason for the problem to be strongly coupled (see section 4.2). In the models of this work this feedback is incorporated through the concept of the effective porosity using the following relation (Darcis (2013) [12]):

$$\phi_{eff} = \frac{\phi_0 + \text{div}(u)}{1 + \text{div}(u)}, \quad (2.56)$$

where $\phi_0$ is the initial porosity.
2.5.5 Effective permeability

The change in porosity again leads to a change in permeability, for which the following expression has been implemented (Darcis (2013) [12]):

\[ K_{\text{eff},ij} = K_{ij} \exp \left( \frac{\phi_{\text{eff}}}{\phi_0} - 1 \right) \]  

(2.57)

2.5.6 Remarks

As explained in the sections above, in this work the rock is assumed to be a linear elastic and isotropic material. In reality rocks are generally anisotropic and show non-linear and non-elastic behaviour. Guegen and Bouteca (2004) [17] point out that the anisotropy results rather small for most rocks, but that the error introduced by neglecting it can be relatively large. Also, according to Jaeger et al. (2007) [20], many rocks show linear elastic behaviour when exposed to incremental stress changes, which is the case in CO2-injection scenarios. Due to its mathematical simplicity, anisotropic linear elastic rocks are often considered in the modeling of such injection scenarios. The author has in mind that these simplifications can be relatively rough and in case a specific real scenario is sought to simulate, the legitimacy of these assumptions has to be verified preliminary. However, this work focuses more on the spatial model coupling and its consequences on the results and the numerical performance.
Chapter 3
Mathematical foundation

In this chapter, the underlying mathematical concepts of the models of this work are introduced. The main focus is on the description of the numerical methods for the discretization and solution of partial differential equations, whereas in the last two sections further mathematical methods used in this work are presented.

The aim of numerical modeling is a reproduction of the physics. However, the solution to the equations that describe the physics is of infinite space and needs to be approximated by a space of finite dimension. In this work, two different schemes have been used for the spatial discretization in the models, both the standard Galerkin finite element method and the Box Method. Their derivation for the differential equation of a general master balance law will be outlined in section 3.2.

The general master balance law for a quantity $\psi$ from equation (2.17) can be rewritten into a simpler form combining the second term on the left side and the first term on the right side of the equation to a new flux term $F$, neglecting the production term and defining $e = \rho \psi$. Furthermore, the primary variable $u$ is introduced for which the equation is solved. That leads to:

$$\frac{\partial e(u)}{\partial t} + \text{div} F(u) - q = 0.$$ (3.1)

3.1 Function spaces

Before the derivation is outlined, the in this context appearing function spaces should be presented and defined. A fundamental function space for the formulation of finite element methods is the Sobolev space $\mathcal{H}^1$. 

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### The Sobolev space \( \mathcal{H}^1 \)

Let \( \Omega \subset \mathbb{R}^n \) be the considered domain, then the Sobolev space is defined as:

\[
\mathcal{H}^1 = \left\{ f : \Omega \to \mathbb{R} \mid \int_{\Omega} f^2 \, d\Omega < \infty, \int_{\Omega} \nabla f^2 \, d\Omega < \infty \right\},
\]

(3.2)

It is thus required that both the squared function, as well as its squared derivatives, are bounded. The inner product for two functions \( f, g \in \mathcal{H}^1 \) is defined as:

\[
(f, g)_{\mathcal{H}^1}(\Omega) = \int_{\Omega} f(x)g(x) + \nabla f(x) \cdot \nabla g(x) \, d\Omega,
\]

(3.3)

where \( f, g : \Omega \to \mathbb{R} \). It can now be defined the \( \mathcal{H}^1 \)-norm:

\[
\|f\|_{\mathcal{H}^1} = \sqrt{(f,f)_{\mathcal{H}^1}}.
\]

(3.4)

The Sobolev space thus contains all functions \( f \) on \( \Omega \) for which the \( \mathcal{H}^1 \)-norm is finite. In finite element calculations, the test and basis functions are usually chosen to be in \( \mathcal{H}^1 \) (see section 3.2). However, the two function spaces have to be specified in order to be able to handle the Dirichlet boundary conditions, which are therefore also called essential boundary conditions. For the solution \( u \in \mathcal{V}^d \) and a test function \( W \in \mathcal{V}^0 \) it must hold:

\[
\mathcal{V}^d(\Omega) = \left\{ u \in \mathcal{H}^1(\Omega) : u = d \quad \text{on} \quad \Gamma_D \right\},
\]

\[
\mathcal{V}^0(\Omega) = \left\{ W \in \mathcal{H}^1(\Omega) : W = 0 \quad \text{on} \quad \Gamma_D \right\}.
\]

(3.5)

Furthermore \( \mathcal{V}^0 = \mathcal{V}^d \) for \( d = 0 \). In other words, the test functions have to vanish and the basis functions have to take the prescribed value on Dirichlet boundaries. Neumann boundaries by contrast emerge naturally during the derivation of the variational formulation (section 3.2) and a further specification of the test or basis functions is not required. They are thus also called natural boundary conditions.

### The \( \mathcal{C}^0 \)-space

\( \mathcal{C}^0 \) is a linear space that contains all continuous functions on \( \Omega \) with non necessarily continuous first order derivatives:

\[
\mathcal{C}^0(\Omega) = \left\{ f : \Omega \to \mathbb{R} \mid f \text{ is continuous on } \Omega \right\}.
\]

(3.6)

The linearity arises from the relationship

\[
\alpha f + \beta g \in \mathcal{C}^0(\Omega), \quad \text{for any } \alpha, \beta \in \mathbb{R} \text{ and } f, g \in \mathcal{C}^0(\Omega).
\]

(3.7)
In this work, $C^0$-Lagrange polynomials are used for the basis functions in both of the implemented spatial discretization schemes. In the introduced form (section 3.2) they are members of $H^1$.

### 3.2 Spatial discretization

For the solution of equation (3.1) for the unknown $u$, initial and boundary conditions need to be assigned. With respect to the initial conditions, the values for $u$ have to be set for the whole domain. On Dirichlet boundaries the values for $u$ are set to $u = \bar{u}$ and on Neumann boundaries the Flux $F \cdot n = F_N$ is prescribed.

#### 3.2.1 Strong formulation

The above mentioned correlations define the so called strong formulation of the problem:

**Problem 3.2.1**

Find $u$ such that

\[
\frac{\partial e(u)}{\partial t} + \text{div} F(u) - q = 0 \quad \text{in } \Omega,
\]

\[
u = \bar{u} \quad \text{on } \Gamma_D,
\]

\[
F \cdot n = F_N \quad \text{on } \Gamma_N.
\]

#### 3.2.2 Variational formulation

Multiplication of equation 3.1 with a test function $W \in V^0$ and integration over a part of the domain $G \subset \Omega$ leads to the variational formulation:

\[
\int_G W \frac{\partial e(u)}{\partial t} \, dG + \int_G W \text{div} F(u) \, dG - \int_G W q \, dG = 0.
\]

Equation 3.9 can now be transformed integrating by parts and applying the Green-Gaussian integral rule on the second term:

\[
\int_G W \frac{\partial e(u)}{\partial t} \, dG + \int_{\Gamma_G} W F(u) \cdot n \, d\Gamma_G
\]

\[
- \int_G \nabla W \cdot F(u) \, dG - \int_G W q \, dG = 0.
\]

The variational formulation of the problem can now be phrased:
Problem 3.2.2
Find $u \in \mathcal{V}^d(G)$ such that

$$
\begin{align*}
\int_G W \frac{\partial e(u)}{\partial t} \, dG &+ \int_{\Gamma_G} W \mathbf{F}(u) \cdot \mathbf{n} \, d\Gamma_G \\
- \int_G \nabla W \cdot \mathbf{F}(u) \, dG &- \int_G W \mathbf{q} \, dG = 0 \quad \forall W \in \mathcal{V}^0(G).
\end{align*}
$$

(3.11)

3.2.3 Discrete formulation

In the following step, the introduced vector spaces have to be approximated by the subspaces $\mathcal{V}^d_h \subset \mathcal{V}^d$, $\mathcal{V}^0_h \subset \mathcal{V}^0$ of finite dimension in order to transform the variational formulation into a finite dimensional system of equations. For this purpose the domain is discretized by dividing it into a mesh of non-overlapping elements. These elements can be of various shape, for example, triangles and rectangles for two-dimensional grids or tetrahedra and hexahedra for three-dimensional grids. The vector spaces are approximated by a set of polynomials that are defined by the values on the vertices of the mesh. The degree of the polynomials for the basis functions is chosen such that they can adequately describe the terms that appear in the governing equations. In this work, $C^0$-Lagrange polynomials are used (see section 3.1). Furthermore, the values for the basis functions $N_j$ are 1 on node $j$ and 0 on every other node. Figure 3.1 illustrates the choice of the test and basis functions for the standard Galerkin finite element and the box method, the two schemes that have been used in this work. Note that the basis functions are chosen identical in both schemes (figure 3.1b).

![Illustration](image)

Figure 3.1: Illustration of the test (a) and basis functions (b) for the standard Galerkin finite element and the box method
The solution can now be approximated by the trial solution \( \tilde{u} \), which is a function of the values at the nodes of the mesh \( \hat{u}_j \) and the corresponding basis functions \( N_j \):

\[
\tilde{u} = \sum_{j=0}^{n} N_j \hat{u}_j,
\]  

(3.12)

where \( n \) is the number of nodes in the domain. The further transformation of the variational formulation into the discrete form is conducted differently for the two methods, based on the choice of the test functions.

**Standard Galerkin Finite Element Method**

In finite element schemes the integration is performed over the entire domain \( \Omega \). The variational formulation thus reads:

\[
\int_{\Omega} W \frac{\partial e(u)}{\partial t} \, d\Omega + \int_{\Gamma_{\text{DN}}} W F(u) \cdot n \, d\Gamma_{\text{DN}} \\
- \int_{\Omega} \nabla W \cdot F(u) \, d\Omega - \int_{\Omega} W q \, d\Omega = 0.
\]  

(3.13)

Note that the surface integral in equation (3.13) only consists of the Neumann boundary, which arises from the fact, that the test functions are required to vanish on those parts of the boundary where \( u \) is known, i.e. on the dirichlet boundary (see section (3.1)). The second term in equation (3.13) can therefore be substituted by the imposed Neumann boundary conditions \( F_N \) (see strong formulation, equation (3.8)). The discrete form of the equation can now be formulated:

**Problem 3.2.3a**

*Find\( \tilde{u} \in V^d_h(\Omega) \)* such that

\[
\int_{\Omega} W \frac{\partial e(\tilde{u})}{\partial t} \, d\Omega + \int_{\Gamma_{\text{DN}}} W F_N \cdot n \, d\Gamma_{\text{DN}} \\
- \int_{\Omega} \nabla W \cdot F(\tilde{u}) \, d\Omega - \int_{\Omega} W q \, d\Omega = 0 \quad \forall W \in V^0_h(\Omega).
\]  

(3.14)

For the standard Galerkin approach, which is used in this work, the test functions are chosen equally to the shape functions (\( W = N \), see figure 3.1). It is also important to keep in mind, that since the integral is evaluated over the whole model domain, this method is not locally, but only globally mass conservative. A big advantage of this method and the reason for it to be used in a wide range of applications is the possibility to model unstructured grids and therefore to map complex domains. With respect to the solution of the integral form, equation (3.14), in the models of this work the integrations are performed using a Gauss quadrature rule based on eight Gaussian points, which is provided by the numerical toolbox DUNE (see section 4.3, Bastian et al. (2008) [3, 2]).
Box Method

The Box method (Helmig (1997) [18]) belongs to the subdomain collocation methods and is locally mass conservative. It can be classified as a node-centered finite volume scheme based on the finite element method. The finite volumes of the box method are constructed using a finite element mesh, connecting the midpoints of the element faces with the barycenters of the elements. One of these finite volumes or boxes belongs to one node of the finite element grid, whereas one finite element contains parts of different boxes called sub control volumes. Figure 3.2 illustrates one box, created around the node \( i \), and its respective sub control volumes.

The integration is now performed over a box \( B \), which means \( G = B \) with respect to equation (3.10):

\[
\int_B W \frac{\partial e(u)}{\partial t} \, dB + \int_{\Gamma_B} W \mathbf{F}(u) \cdot \mathbf{n} \, d\Gamma_B - \int_B \nabla W \cdot \mathbf{F}(u) \, dB - \int_B W \, q \, dB = 0. \tag{3.15}
\]

For the box method, piecewise constant test functions are chosen, which are only non-zero within the considered box (see figure 3.1):

\[
W = \begin{cases} 
1, & \text{if } x \in B \\
0, & \text{if } x \notin B. 
\end{cases} \tag{3.16}
\]

As a result, \( W \) is always 1 inside the box and \( \nabla W = 0 \):

\[
\int_B W \frac{\partial e(u)}{\partial t} \, dB + \int_{\Gamma_B} \mathbf{F}(u) \cdot \mathbf{n} \, d\Gamma_B - \int_B W \, q \, dB = 0. \tag{3.17}
\]

Furthermore, a mass lumping technique (Huber (1999) [19]) can be applied to the storage and the source/sink term (first and third term). The proceeding is here shown for the storage term of the box \( i \), in which is first inserted the expression (3.12) for the trial solution \( \tilde{u} \) and then evaluated the integral using a Gauss quadrature rule with \( n_G \) points and their respective coordinates \( p_k \) and weighting factors \( \alpha_k \):

\[
\int_{B_i} W_i \frac{\partial e(\sum_{j=1}^{n} N_j \tilde{u}_j)}{\partial t} \, dB_i = \sum_{k=1}^{n_G} \sum_{j=1}^{n} \alpha_k W_i(p_k) N_j(p_k) \frac{\partial e(\tilde{u}_j)}{\partial t}. \tag{3.18}
\]

The product \( W_i(p_k) N_j(p_k) \) describes the influence of the neighboring nodes on node \( i \). Mass lumping now means, that the influences of the surrounding nodes on the storage term of a node \( i \) are not considered, but instead replaced by the value at the considered node. If this approach is inserted into equation (3.18) and it is further considered that \( W_i = 1 \)
inside the box $i$ and therefore $\int_{B_i} W_i \, dB_i = V_i$, it results:

$$\sum_{k=1}^{n_g} \sum_{j=1}^{n} \alpha_k W_i(p_k) N_j(p_k) \frac{\partial e(\hat{u}_i)}{\partial t} = \sum_{k=1}^{n_g} \alpha_k W_i(p_k) \frac{\partial e(\hat{u}_i)}{\partial t} = V_i \frac{\partial e(\hat{u}_i)}{\partial t}. \quad (3.19)$$

As a consequence of that, the storage term is, like in finite volume schemes, a constant value for the whole box. According to Celia et al. (1992) \[10\], mass lumping reduces the occurrence of non-physical oscillations in the solution. The same procedure can also be performed on the source/sink term and the discrete formulation of the problem for the box method can be formulated:

**Problem 3.2.3b**

Find $\tilde{u} \in \mathcal{V}^d_h$ such that

$$V_B \frac{\partial e(\tilde{u}_B)}{\partial t} + \int_{\Gamma_B} \mathbf{F}(\tilde{u}) \cdot \mathbf{n} \, d\Gamma_B - V_B q_B = 0. \quad (3.20)$$

Because of the creation of a secondary mesh, based on the finite element mesh, the box method is applicable to unstructured grids. Furthermore, since the integration is performed over the different boxes instead of the whole domain and the fluxes over the box surfaces are explicitly evaluated (second term in equation (3.20)), the scheme guarantees local mass conservation. These two attributes make this method very attractive for fluid flow calculations.

The surface integral from equation (3.20) is approximated by the sum of the fluxes over the sub control volume faces. This is done by evaluating the fluxes at the integration points on the different sub control volume faces and their multiplication with the respective surface area. One integration point for one subcontrol volume face is exemplarily depicted in figure 3.2.

Figure 3.2: Illustration of a box and sub control volumes of node $i$ in the FE mesh
3.3 Time discretization

For the discretization of the time derivatives in the storage terms of the implemented equations (see section 4.2), a fully implicit Euler scheme has been applied. It is a finite difference method of first order, in which for a time step size \( \Delta t \), all the terms are evaluated for the new time level \( t + \Delta t \). Furthermore, it is unconditionally stable and can therefore be applied to the complex task of modeling two phase flow coupled with linear elastic deformations in porous media. For a general differential equation

\[
\frac{\partial u}{\partial t} - f(u) = 0, \quad (3.21)
\]

the application of the implicit Euler scheme on the time derivative leads to:

\[
\frac{\partial u}{\partial t} = \frac{u^{t+\Delta t} - u^t}{\Delta t} = f(u^{t+\Delta t}). \quad (3.22)
\]

After the insertion of this approach to the variational formulation of the general master balance law for the box method (equation (3.20)), it now reads:

\[
V_i e(\hat{u}_i)^{t+\Delta t} - e(\hat{u}_i)^t + \int_{\Gamma_{B_i}} F(\hat{u})^{t+\Delta t} \cdot n \, d\Gamma_{B_i} - V_i q_i^{t+\Delta t} = 0. \quad (3.23)
\]

Remarks

The application of the numerical methods for the spatial and temporal discretization presented in this and the previous section on a differential equation results in a system of equations of size \( m = u \cdot n \), where \( u \) is the number of unknowns and \( n \) is the number of nodes that has been used to spatially discretize the domain. Note that the above presented derivation was outlined for a scalar property and thus a single equation and a single unknown, but the property could also be vector valued and/or the to be modeled physical processes could be described by a coupled set of equations. In any case, the resulting system of equations can be rearranged into a root finding problem

\[
F(u) = 0, \quad (3.24)
\]

and formulated in matrix form

\[
A u = 0, \quad (3.25)
\]

where \( u \) is the vector of unknowns of size \( m = u \cdot n \) and \( A \) is the coefficient matrix of the linear equation system of size \( (m \times m) \). For linear systems, the matrix \( A \) can be assembled directly and only depends on the test and basis functions. Non-linear systems first have to
be linearized by e.g. a Newton-Raphson method (section 3.4). The matrix \( A \) then contains the derivatives \( A_{ij} \) of equation \( i \) with respect to \( u_j \) and \( u \) converts into \( \Delta u \), i.e. the increment of the vector of unknowns.

### 3.4 Newton-Raphson method

As already mentioned, the Newton-Raphson method can be used to linearize the system of equations resulting from the discretization of non-linear differential equations and thus forms a crucial part in numerical simulations. The equations of the models of this work (see section 4.2) incorporate non-linear dependencies and thus a Newton-Raphson method is executed in each time integration (see section 4.3.2). The Newton-Raphson method is here presented in a more general manner, not referring to discretization schemes, since it is a universal method for the solution of non-linear equation systems.

Consider a system of \( n \) non-linear equations \( f_i(x_1, x_2, ..., x_n), \ i \in \{1, 2, ..., n\} \) with \( x_n \) variables. In vector notation it can be written as:

$$f(x) = 0. \quad (3.26)$$

The system can be linearized through a Taylor series expansion of \( f \) at \( x = \tilde{x} \) and truncation after \( O(1) \):

$$f_{\text{lin}}(\tilde{x} + \Delta x) \approx f(\tilde{x}) + \left. \frac{\partial f(x)}{\partial x} \right|_{x=\tilde{x}} \Delta x, \quad (3.27)$$

where the Jacobian matrix

$$J(x) = \frac{\partial f(x)}{\partial x} \quad (3.28)$$

appears. It describes the change of \( f \) or rather each \( f_i, \ i \in \{1, 2, ..., n\} \) due to changes in the unknowns \( x_n \), and is thus of size \( n \times n \). It can be approximated numerically at \( x = \tilde{x} \) by e.g. a central difference method:

$$J_{ij} = \frac{\partial f_i}{\partial x_j} = \frac{f_i(\tilde{x}_1, ..., \tilde{x}_j + \delta x_j, ..., \tilde{x}_n) - f_i(\tilde{x}_1, ..., \tilde{x}_j - \delta x_j, ..., \tilde{x}_n)}{2 \cdot \delta x_j}. \quad (3.29)$$

Here, \( \delta x_j = \epsilon \cdot \tilde{x}_j \) is a small increment of the unknown \( x_j \), with e.g. \( \epsilon = 10^{-8} \). It is now started at an initial guess \( \tilde{x}_0 \) for the solution and the linear approximation of the system, equation \( (3.27) \), is solved for the increment \( \Delta x \)

$$f_{\text{lin}}(\tilde{x}_0 + \Delta x) = 0 \quad \rightarrow \quad \Delta x = -J^{-1}(\tilde{x}_0) f(\tilde{x}_0). \quad (3.30)$$
The new solution vector

\[ \tilde{x}_1 = \tilde{x}_0 + \Delta x \]  

(3.31)

is now taken as a better approximation and the last step is repeated \( k \) times until the
defect falls below a previously defined value:

\[ ||f(\tilde{x}_k)||_2 < \epsilon, \]  

(3.32)

where the defect is the Euclidean vector norm of the function vector:

\[ ||f(\tilde{x}_k)||_2 = \sqrt{\sum_{m=1}^{n} [f_m(\tilde{x})]^2}. \]  

(3.33)

The vector \( x_k \) is thus the solution to the non-linear system of equations.

### 3.5 Gauss-Newton algorithm

The Gauss-Newton algorithm is used to solve non-linear least squares problems and in
this work especially for a non-linear least squares fitting (see section 4.6.2).

**The problem**

For a given set of \( n \) pairs of data \( (x_i, y_i), i \in \{1, 2, ..., n\} \), find the \( m \) parameters
\( \beta_j, j \in \{1, 2, ..., m\} \) of the model curve \( f(x, \beta) \) so that the sum of the squares of the
deviations

\[ S(\beta) = \sum_{i=1}^{n} [y_i - f(x_i, \beta)]^2 = ||y - f(x, \beta)||_2^2 \]  

(3.34)

becomes minimal, or in other words:

*Find \( \beta \) such that*

\[ \nabla S(\beta) = \frac{\partial S(\beta)}{\partial \beta} = 0. \]  

(3.35)
3.5 Gauss-Newton algorithm

The solution

In a first step, the model function \( f(x, \beta) \) is again linearized with respect to the parameter vector \( \beta \) in a Taylor series expansion around an initial guess \( \beta_0 \) and truncation after \( \mathcal{O}^1 \):

\[
f(x, \beta_0 + \Delta \beta) \approx f(x, \beta_0) + J(\beta)|_{\beta = \beta_0} \Delta \beta,
\]

where \( J \) is again the Jacobian matrix

\[
J(\beta) = \frac{\partial f(x, \beta)}{\partial \beta}
\]

Insertion of equation (3.36) into equation (3.35) yields

\[
\nabla S(\beta) \approx [y - f(x, \beta_0) - J(\beta_0)\Delta \beta] J(\beta_0) = 0
\]

and after rearranging:

\[
J(\beta_0)^T J(\beta_0) \Delta \beta = J(\beta_0)^T [y - f(x, \beta_0)].
\]

The different data points can furthermore be weighted, introducing the weighting matrix \( W \), in order to give more importance to some of them and to enforce the curve to relatively fit better on those points:

\[
J(\beta_0)^T W J(\beta_0) \Delta \beta = J(\beta_0)^T W [y - f(x, \beta_0)].
\]

This set of linear equations can now be solved for the increment \( \Delta \beta \) and the new update for \( \beta \)

\[
\beta_1 = \beta_0 + \Delta \beta
\]

is used as a new guess and the algorithm is repeated \( k \) times until the increment becomes sufficiently small:

\[
||\Delta \beta_k||_2 < \epsilon.
\]

The parameter vector \( \beta_k \), then contains the parameters for which the model curve \( f(x, \beta) \) best fits the given data.
3.6 Theis equation

In 1935, Charles Vernon Theis (* 03/27/1900 in Newport, Kentucky, USA; † 07/31/1987) presented an analytical solution for the transient drawdown in an infinite uniform confined aquifer provoked by a pumping well (Theis (1935) [28]). When he had faced the task of finding a solution to the problem, he recognized the analogy to the theory of heat conduction and therefore consulted his friend and mathematician Clarence Lubin of the University of Cincinnati. He in turn referred to Horatio Scott Carlslaw’s solution to the time-dependent radial heat flow from a line source (Carlslaw (1921) [9]), on the basis of which C.V. Theis then developed an equation for the calculation of the drawdown, which should look very similar.

In order to derive an analytical solution to the problem of groundwater flow to a pumping well, a few prior assumptions have to be made:

\( (A1) \) Prior to pumping, the piezometric level is horizontal

\( (A2) \) The aquifer is confined and has infinite horizontal extent

\( (A3) \) The aquifer is homogeneous, isotropic and of uniform thickness

\( (A4) \) The well is fully penetrating the aquifer

\( (A5) \) The well is pumped at a constant rate

\( (A6) \) The well diameter is infinitesimally small so that well storage is neglectable

**Governing equation**

The equation that describes the problem is the groundwater flow equation, which in cylindrical coordinates and for the above assumptions can be expressed as (formulated for the drawdown instead of the piezometric head):

$$\frac{\partial^2 s}{\partial r^2} + \frac{1}{r} \frac{\partial s}{\partial r} = \frac{S}{T} \frac{\partial s}{\partial t}. \tag{3.43}$$

Here, \( s(r,t) \) is the drawdown of the piezometric head, \( T \) denotes the transmissivity, \( S \) the storativity of the aquifer and \( r \) is the radial distance to the pumping well. The boundary conditions for the Theis problem are:

$$s \to 0 \quad \text{for} \quad r \to \infty, \ t \geq 0 \tag{3.44}$$

and

$$-2\pi r T \frac{\partial s}{\partial r} = Q \quad \text{for} \quad r \to 0, \ t > 0, \tag{3.45}$$
where $Q$ is the constant extraction rate (A5) of the well. The initial condition is given by

$$s = 0 \text{ for } t = 0. \quad (3.46)$$

As seen in the boundary condition at the well, the validity of Darcy’s law is assumed (see section 2.4). In fact, a number of further assumptions are included in equation (3.43), which are as follows:

(A7) Slow flow velocities (Darcy’s law applicable)

(A8) The solid matrix is incompressible, i.e. it experiences no changes due to pressure changes

(A9) Incompressible water ($\rho_w = \text{const.}$)

(A10) No changes in external loads on the aquifer

(A11) isotropic, scalar hydraulic conductivity ($K$, included in $T$ and $S$)

The equations (3.43) - (3.46) correspond to a formal description of the problem. In the following the derivation of the Theis solution to this problem will be outlined.

**Derivation of the Theis Equation**

For the search of a general solution to the Theis problem, in a first step an adequate dimensionless variable has to be found. The drawdown $s$ will be a function of $Q$, $r$, $t$ as well as the aquifer parameters $T$ and $S$. But, as $Q$ only appears in the boundary condition and $S$ itself is dimensionless, these two variables does not have to be included in the new variable. However, here it is already known that the Theis equation is formulated on the basis of the dimensionless variable

$$u = \frac{r^2 S}{4tT}. \quad (3.47)$$

A different choice could also be made and would lead to a similar result. Equation (3.43) can now be rewritten applying the chain rule of differentiation on the appearing derivatives

$$\frac{\partial s}{\partial r} = \frac{\partial s}{\partial u} \frac{\partial u}{\partial r}, \quad (3.48)$$

$$\frac{\partial s}{\partial t} = \frac{\partial s}{\partial u} \frac{\partial u}{\partial t}. \quad (3.49)$$

which gives the relations:
3.6 Theis equation

\[ \frac{\partial s}{\partial r} = \frac{rS}{2tT} \frac{\partial s}{\partial u}, \quad (3.50) \]

\[ \frac{\partial s}{\partial t} = -\frac{r^2S}{4t^2T} \frac{\partial s}{\partial u}, \quad (3.51) \]

\[ \frac{\partial^2 s}{\partial r^2} = -\left( \frac{rS}{2tT} \right)^2 \frac{\partial^2 s}{\partial u^2} + \frac{S}{2tT} \frac{\partial s}{\partial u}. \quad (3.52) \]

Note that for the second order derivative Faà di Bruno’s formula has been used to find the respective chain rule. Inserting the above relations into the groundwater flow equation (3.43) yields:

\[ u \frac{\partial^2 s}{\partial u^2} + (1 + u) \frac{\partial s}{\partial u} = 0. \quad (3.53) \]

After defining \( s' = ds/du \) and after the separation of variables, the equation can further be rewritten to

\[ \frac{ds'}{s'} = -\left( \frac{1}{u} + 1 \right) \, du \quad (3.54) \]

and integrated

\[ \ln(s') = C - (\ln u + u), \quad (3.55) \]

with \( C \) being a constant. Taking the exponential of both sides of the equation gives

\[ s' = C_1 \frac{\exp(-u)}{u}, \quad (3.56) \]

which can then again be integrated to the general solution

\[ s = C_1 \int_{0}^{u} \frac{\exp(-x)}{x} \, dx + C_2, \quad (3.57) \]

where \( C_1 \) and \( C_2 \) are constants and \( x \) is the variable of integration. The constant \( C_2 \) can be evaluated through the boundary condition (3.44) and the initial condition (3.46). For \( t \to 0 \) and \( r \to \infty \) it is \( u \to \infty \), so the two conditions result in an expression for the parameter \( C_2 \):

\[ C_2 = -C_1 \int_{0}^{\infty} \frac{\exp(-x)}{x} \, dx. \quad (3.58) \]
3.6 Theis equation

The constant $C_1$ can be found through the well boundary condition (3.45) and equation (3.56), using that $u \to 0$ for $r \to 0$ and that $\frac{ds}{dr} = \frac{du}{dr} = \frac{2u}{r} s'$:

$$C_1 = -\frac{Q}{4\pi T}.$$  \hspace{1cm} (3.59)

The Theis solution to the problem can now be found by inserting the expressions for the two constants in equation (3.57) and combining the two integrals:

$$s = \frac{Q}{4\pi T} \int_{u}^{\infty} \frac{\exp(-x)}{x} \, dx = \frac{Q}{4\pi T} w(u).$$  \hspace{1cm} (3.60)

The integral in equation (3.60) is the exponential integral function which is often referred to as the *Theis well function* $w(u)$ by groundwater hydrologists. It can be evaluated through the infinite series

$$w(u) = -\gamma - \ln u - \sum_{n=1}^{\infty} \frac{(-1)^n u^n}{n! n},$$  \hspace{1cm} (3.61)

where $\gamma = 0.5772156649...$ is the *Euler-Mascheroni* constant. According to Tseng et al. (1998) [30], the series (3.61) converges for any finite value of $u$, although it converges very slowly for large ones.

Jacob and Cooper (1946) [11] stated, that for $u \leq 0.02$, an adequate approximation of the Theis well function is given by simply evaluating the two first terms of equation (3.61):

$$w(u) \approx -\gamma - \ln u = \ln \left( \exp \left( -\gamma \right) \right) - \ln u = \ln \left( \frac{\exp \left( -\gamma \right) u}{u} \right).$$  \hspace{1cm} (3.62)

Inserting this and the definition of $u$ into equation (3.60) leads to a simplified expression for the drawdown:

$$s = \frac{Q}{4\pi T} \ln \left( \frac{2.25 T t}{r^2 S} \right) \quad \text{for} \quad \frac{r^2 S}{4t T} \leq 0.02.$$  \hspace{1cm} (3.63)
Chapter 4
Model concept

4.1 Problem description and motivation

This work aims for the simulation of CO₂ injection scenarios in deep saline aquifers under the application of spatial model coupling. As explained in section 2.1 numerous physical phenomena emerge in conjunction with such an injection. However, depending on the temporal and spatial scales, some of these processes might be neglectable. Both the propagation of the pressure as well as of the stresses in the rock matrix are described by elliptic partial differential equations, which means the information originating from a deflection of the system at a certain point, spreads in all directions. Furthermore, the system’s response
4.1 Problem description and motivation

to such a deflection is of infinite space, with the information traveling at the speed of sound. However, solid and fluid exhibit different characteristics for the decay of the deflection. As it can be seen in the governing equations that will be presented in section 4.2 with respect to the stresses this decay depends on the two lamé parameters and thus effectively on Young’s modulus and the poisson ratio. With respect to the pressure, it depends on the permeability of the rock, which is of several orders of magnitude smaller. This means that the pressure buildup caused by the injection might be negligibly small in regions distant to the injection well, whereas the occurring displacements are considerable.

With respect to the modeling of such injection scenarios, it results that the spatial scales on which the boundary conditions influence the model’s solution to the problem are of different size. The fluid pressure and thus the flow processes are influenced by the boundary conditions on smaller scales than the rock’s mechanical response to the injection. From the mechanical point of view, the domain has to be chosen larger than for a simply hydraulical model in order for the domain boundaries to have a smaller effect on the resulting displacement field. It thus arises the idea of neglecting the flow processes in distances where for the considered time span no important pressure buildup will be observable, but nevertheless calculating the displacement field in order to fully capture the effects the injection imposes on the reservoir and its feedback on the flow field.

For this reason, a purely mechanical model is solved in the outer parts of the domain in greater distances to the injection well, whereas the domain adjacent to the well is described by a linear elastic model coupled with a two-phase flow model. In the following, these two models and domains will be referred to as the el-model, the el-subdomain and the el2p-model and el2p-subdomain, respectively. An illustration of the problem is given in figure 4.1. Since in the el-model the two phase flow is not incorporated, boundary conditions at the interface between the two subdomains have to be defined for the mass balance equations of CO$_2$ and brine. Various approaches for the modeling of the interface have been implemented and tested in this work and are presented in chapter 4.6. Note that the algorithms have only been programmed for radial grids with hexahedral elements and a horizontally layered structure so far, as such a grid has been used for all the simulations presented in this work (see section 4.5). Furthermore, note that the presented models imply very pragmatic approaches, which makes them unsuitable for complex geometries or heterogeneous domains. The author had this in mind while developing the models, as well as the fact that they do not provide elaborate mathematical derivations.

\footnote{It should be stated that the domain would have to be chosen extremely large to have a neglectable influence of the boundaries}
4.2 Mathematical models

Each of the implemented models requires a distinct mathematical description, that has to be derived individually. Generally, for the description of a body under the influence of thermomechanical stress, one can make use of the fundamental balance equations for the system’s mass, linear momentum, angular momentum, the total energy and the entropy. The derivation has to be executed according to the regarded problem and by formulating adequate assumptions. In the following sections the derivation of the individual models of this work will be outlined. Please note that a detailed description of the concept behind the introduced pressure $p_{el}$ appearing in the $el$-model will be given in chapter 4.6.

4.2.1 A linear elastic two-phase model: the el2p-model

The system consists of three phases, the two fluid phases water and CO$_2$ and the solid phase of the rock. Before further deriving the governing equations, a few assumptions are made in order to simplify the system:

(A1) All participating solid materials are consolidated in a single solid phase $s$

(A2) Small deformations of the solid (application of small deformation theory valid)

(A3) Incompressible solid matrix and brine phase ($\rho_s = \text{const.}$, $\rho_w = \text{const.}$)

(A4) Isothermal conditions (solving the energy balance is not required)

(A5) Quasi stationary conditions (inertia forces are neglected, i.e. $\rho_s \dot{v}_s = 0$)

(A6) All the participating phases are immiscible within each other.

Governing equations

For the derivation of the system of equations that describes the problem, one can make use of the mass and the momentum balance equations for all of the three participating phases. However, the mass balance equation of the solid phase is not solved explicitly in the presented model, but included through the relation for $\phi_{eff}$ as given in equation (2.56). Furthermore, the momentum balance equations of the fluid phases are included in the form of the standard Darcy multiphase approach, i.e. equation (2.34). The mass balance equations can be derived from equation (2.17) by inserting $\psi = n_\alpha = \phi S_\alpha$ and by describing the fluid’s movement relative to the solid,

$$v_\alpha = (v_\alpha - v_s) + v_s,$$

(4.1)
which gives

\[
\frac{\partial (\phi_{\text{eff}} \rho_{\alpha} S_{\alpha})}{\partial t} + \text{div} (\phi_{\text{eff}} \rho_{\alpha} S_{\alpha} (\mathbf{v}_{\alpha} - \mathbf{v}_{s})) + \text{div} (\phi_{\text{eff}} \rho_{\alpha} S_{\alpha} \frac{\partial \mathbf{u}}{\partial t}) = q_{\alpha}, \quad \alpha \in \{w, \text{CO}_2\}.
\]  

(4.2)

In the above equation the Darcy velocity

\[
\mathbf{v}_{D_{\alpha}} = \phi_{\text{eff}} S_{\alpha} (\mathbf{v}_{\alpha} - \mathbf{v}_{s})
\]  

(4.3)

can be identified. With respect to the momentum balance equation of the porous medium, one obtains (using assumption (A5)) in accordance to equation (2.25):

\[
\text{div} (\sigma_{\text{eff}}) + \rho_{b} \mathbf{g} = 0.
\]  

(4.4)

The stress in the porous medium is expressed through the effective stress (see section 2.5.3)

\[
\sigma_{\text{eff}} = \sigma_{s} - p_{\text{eff}} I
\]  

(4.5)

and furthermore the bulk density \( \rho_{b} \) comes into play, which is defined as:

\[
\rho_{b} = \phi_{\text{eff}} (S_{\text{CO}_2} \rho_{n} + S_{w} \rho_{w}) + (1 - \phi_{\text{eff}}) \rho_{s}.
\]  

(4.6)

Since a linear elastic material law is used, the following linearization can be applied to the effective stress tensor by subtracting the initial state (subscript 0):

\[
\sigma_{\text{eff}} - \sigma_{\text{eff,0}} = \sigma_{s} - \sigma_{s,0} - (p_{\text{eff}} - p_{\text{eff,0}}) I, \\
\Delta \sigma_{\text{eff}} = \Delta \sigma_{s} - \Delta p_{\text{eff}} I.
\]  

(4.7)

The linearization of the momentum balance equation allows an easier implementation of the initial and boundary conditions. Regarding the initial conditions, the effective stress change \( \Delta \sigma_{\text{eff}} \) and thus the solid displacement \( \mathbf{u} \) can be set to zero for the whole domain. In contrast, if the full momentum balance is solved, one has to take into account the prevailing in-situ stress field and effective stress field resulting from the overburden. The corresponding spatial distribution of the displacement then has to be determined by solving the momentum balance equation in a pre-processing step (Darcis (2013) [12]).

The linearized form of equation (4.4) reads as follows:

\[
\text{div} (\Delta \sigma_{\text{eff}} - \Delta p_{\text{eff}} I) + \Delta \rho_{b} \mathbf{g} = 0.
\]  

(4.8)
The change in bulk density

\[ \Delta \rho_b \mathbf{g} = \Delta \phi (S_{CO_2} \rho_n + S_w \rho_w) \mathbf{g} + \phi \Delta (S_{CO_2} \rho_n + S_w \rho_w) \mathbf{g} + \Delta (1 - \phi) \rho_s \mathbf{g} + (1 - \phi) \Delta \rho_s \mathbf{g}. \]  

(4.9)

can further be simplified under the assumption of small porosity changes \( \Delta \phi \approx 0 \), \( \Delta (1 - \phi) \approx 0 \) and an incompressible solid matrix \((A3)\). This cancels out the first, third and fourth term:

\[ \Delta \rho_b \mathbf{g} = \phi \Delta (S_{CO_2} \rho_n + S_w \rho_w) \mathbf{g}. \]  

(4.10)

Also, the term \( \phi S_{CO_2} \Delta \rho_n \) will result in way smaller values than \( \phi \rho_n \Delta S_{CO_2} \) and is therefore not considered. Moreover, as defined in assumption \((A3)\), the compressibility of the brine phase is neglected. For all the CO\(_2\) injection scenarios that are simulated in this work, the initial saturation is equal to one and thus \( \Delta S_{CO_2} \) becomes \( S_{CO_2} \) and \( \Delta S_w \) becomes \( -S_{CO_2} \):

\[ \Delta \rho_b \mathbf{g} = \phi S_{CO_2} (\rho_n - \rho_w) \mathbf{g}. \]  

(4.11)

It is obtained the linearized momentum balance equation:

\[ \text{div}(\Delta \sigma_{\text{eff}} - \Delta p_{\text{eff}} I) + \phi S_{CO_2} (\rho_n - \rho_w) \mathbf{g} = 0. \]  

(4.12)

**Constitutive equations and supplementary constraints**

For the closure of the system, constitutive equations and constraints are required:

\( (C1) \) Darcy’s law is valid for the fluid velocities (see above)

\[ \rightarrow \mathbf{v}_{D,\alpha} = -\frac{k_{\alpha}}{\mu_\alpha} \mathbf{K} (\nabla p_\alpha - \rho_\alpha \mathbf{g}). \]

\( (C2) \) Linear elastic material behaviour of the rock

\[ \rightarrow \sigma_s = \lambda \text{tr}[\epsilon] \mathbf{I} + 2\mu \epsilon. \]

\( (C3) \) The sum of the saturations has to add up to one

\[ \rightarrow \sum_\alpha S_\alpha = 1 \]  (see section \[2.2.2\]).

\( (C4) \) The pressures are connected via the capillary pressure

\[ \rightarrow p_n = p_w + p_c (S_\alpha) \]  (see section \[2.2.5\]).
All the equations are solved fully coupled in order to capture the mutual interaction. Decoupled solution procedures to the problem exist (Darcis (2013) [12]), however, because of the strong coupling between the different balance equations, it can be described most accurately with a fully coupled approach (Settari et al. (2008) [26]).

After the insertion of the supplementary constraints the system is closed, that means it has to be solved for 5 primary variables. Because of the two constraints \((C3)\) and \((C4)\) one can choose two of them from the two saturations and two fluid pressures. In this work a \(p_w-S_n\) formulation has been used, which means that the water pressure \(p_w\) and the nonwetting phase saturation \(S_{CO_2}\) are chosen as the two primary variables in addition to the displacement vector \(u\). This leads to the strong formulation of the problem as follows, with \(f\) being a normal force acting on the Neumann boundary:

**Problem 4.2.1**

Find \(u\), \(p_w\) and \(S_{CO_2}\) such that

\[
\begin{align*}
\frac{\partial (\phi_{eff} p_w(1-S_{CO_2}))}{\partial t} - \text{div} \left\{ p_w \frac{k_{rw}}{\mu_w} K_{eff} \left( \nabla p_w - \rho_w g \right) + \phi_{eff} p_w (1-S_{CO_2}) \frac{\partial u}{\partial t} \right\} &= 0 \quad \text{in } \Omega, \\
\frac{\partial (\phi_{eff} \rho_n S_{CO_2})}{\partial t} - \text{div} \left\{ \rho_n \frac{k_{rn}}{\mu_n} K_{eff} \left( \nabla (p_w + \rho_c(S_{CO_2})) - \rho_n g \right) + \phi_{eff} \rho_n S_{CO_2} \frac{\partial u}{\partial t} \right\} &= 0 \quad \text{in } \Omega, \\
\text{div}(\Delta \sigma - \Delta p_{eff} I) + \phi S_{CO_2} (\rho_n - \rho_w) g &= 0 \quad \text{in } \Omega, \\
\rho_w &= \bar{p}_w \quad \text{on } \Gamma_D, \\
S_{CO_2} &= \bar{S}_n \quad \text{on } \Gamma_D, \\
u &= \bar{u} \quad \text{on } \Gamma_D, \\
-p_w \frac{k_{rw}}{\mu_w} K_{eff} \left( \nabla p_w - \rho_w g \right) + \phi_{eff} p_w (1-S_{CO_2}) \frac{\partial u}{\partial t} n &= q_w \quad \text{on } \Gamma_N, \\
-\left( \rho_n \frac{k_{rn}}{\mu_n} K_{eff} \left( \nabla (p_w + \rho_c(S_{CO_2})) - \rho_n g \right) + \phi_{eff} \rho_n S_{CO_2} \frac{\partial u}{\partial t} \right) n &= q_n \quad \text{on } \Gamma_N, \\
(\Delta \sigma - \Delta p_{eff} I) n &= f \quad \text{on } \Gamma_N.
\end{align*}
\]

\((4.13)\)
4.2.2 A Linear elastic Model: the el-model

This model aims for the description of the solid’s response to the load imposed by the injection. Further assumptions are made in accordance to section 4.2.1:

(A1) All participating solid materials are consolidated in a single solid phase \( s \)

(A2) Small deformations (application of small deformation theory valid)

(A3) Incompressible solid matrix \( (\rho_s = \text{const.}) \)

(A4) Isothermal conditions (solving the energy balance is not required)

(A5) Linear elastic material behaviour of the rock \( (T = \sigma) \)

(A6) Quasi stationary conditions (inertia forces, i.e. \( \rho_s \dot{v}_s = 0 \)).

**Governing equations**

For the description of the displacements of a solid material, it has to be solved the quasi stationary \( (A5) \) momentum balance equation, which reads:

\[
\text{div}(\sigma_s) + \rho_s g = 0. \tag{4.14}
\]

As explained later in chapter 4.6 for one of the different coupling concepts, a pseudo pressure \( p_{el} \) has been introduced in the el-domain. The introduction of this quantity allows a formulation in effective stresses. Furthermore, a linearization of the equation can again be performed for the linear elastic material law. Under the assumption of an incompressible solid \( (A3) \), it follows the linearized momentum balance equation:

\[
\text{div}(\Delta \sigma_s - \Delta p_{el} I) = 0. \tag{4.15}
\]

Note that for the those coupling concepts presented in chapter 4.6 that do not comprise the introduction of the pseudo pressure \( p_{el} \), the term \( \Delta p_{el} \) vanishes. The respective strong formulation of the problem can now be formulated:

**Problem 4.2.2**

*Find \( u \) such that*

\[
\begin{align*}
\text{div}(\Delta \sigma_s - \Delta p_{el} I) &= 0 \quad \text{in } \Omega, \\
 u &= \bar{u} \quad \text{on } \Gamma_D, \\
 \sigma n &= f \quad \text{on } \Gamma_N.
\end{align*} \tag{4.16}
\]
## 4.2.3 Summary

In the previous sections the equations that describe the physical processes that are aimed to be modeled, were presented. The following table gives an overview over the mathematical models and the respective primary variables.

<table>
<thead>
<tr>
<th>model</th>
<th>equations</th>
<th>primary variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>el2p-model</td>
<td>eq. (4.2), eq. (4.12)</td>
<td>$p_w$, $S_{CO_2}$, $u_x$, $u_y$, $u_z$</td>
</tr>
<tr>
<td>el-model</td>
<td>eq. (4.15)</td>
<td>$u_x$, $u_y$, $u_z$</td>
</tr>
</tbody>
</table>

Table 4.1: The two models and the respective equations and primary variables

## 4.3 Numerical Models

All the simulations have been performed with the numerical toolbox DuMu$^x$ (Flemisch et al. (2011) [16]), which is based on the Distributed and Unified Numerics Environment DUNE (Bastian et al. (2008) [3, 2]). The equations presented in chapter 4.2 were already implemented in Dumux, although the momentum balance equation for the el-model (equation (4.15)) was originally discretized with the Box-Method and had to be reprogrammed to a standard Galerkin finite element method (see section 4.3.1). The reason for this is based on stability problems, i.e. strong pressure oscillations, within the el2p-model, when both the mass balance equations of the fluids and the momentum balance equations for the porous medium are discretized with the box scheme (Darcis (2013) [12]). These could be efficiently reduced by applying an FEM-scheme to the momentum balance equation with and only discretizing the mass balance equations with the box method. Due to the different test functions (see figure 3.1a), the integration domains are different, i.e. span over all the adjacent elements for the finite element, and are restricted to the boxes around nodes for the box method (see figure 3.2). This led to a strong reduction of the pressure oscillations. It is further mentioned in Darcis (2013) [12], that the application of a staggered grid is expected to lead to a further stability increase of the el2p-model. This assumption is based on the work of Kim (2010) [21], where this approach has been used to reduce oscillations that arose from the equal-order approximation of the pressure and the solid displacement in a finite element scheme. A future work could thus be the development of a staggered grid scheme for the el2p-model.

In the following the transition from the mathematical models presented in 4.2 to the numerical models, i.e. to the discretized equations, is outlined and in section 4.3.2 the solution procedure is explained.
4.3 Numerical Models

4.3.1 Discretized Equations

Mass balance equations

As already mentioned, for the discretization of the mass balance equations of the el2p-model, the box method was used. In section 3.2.3, the application of this method combined with a mass lumping technique for the storage and the source/sink term and the fully implicit Euler scheme for the time derivative was presented for a general balance law. The procedure led to the equations (3.20) and (3.23). When performing the same operations on the fluid mass balances (see section 4.2), on the resulting the surface integral

\[- \int_{\Gamma_B} \left( \rho_\alpha \frac{k_{ra}}{\mu_\alpha} \mathbf{K}_{eff} (\nabla \tilde{p}_\alpha - \rho_\alpha \mathbf{g}) + \phi_{eff} \rho_\alpha \tilde{S}_\alpha \frac{\partial \tilde{u}}{\partial t} \right) t^{+\Delta t} \cdot \mathbf{n} d\Gamma_i \]  

(4.17)

a fully upwinding technique is applied to receive stable, non-oscillating solutions (Helmig (1997) [18]). That means that the coefficients for the calculation of the flux are evaluated at the upstream node. The upstream node is found using the total potential of a phase \( \alpha \) at node \( i \)

\[ \hat{\psi}_{\alpha i} := \tilde{p}_{\alpha i} - \rho_{\alpha i} \mathbf{g} \hat{z}_i \]  

(4.18)

in the following way:

\[ \text{upw}(i,j) = \begin{cases} i, & \text{for } (\hat{\psi}_{\alpha j} - \hat{\psi}_{\alpha i}) \leq 0 \\ j, & \text{for } (\hat{\psi}_{\alpha j} - \hat{\psi}_{\alpha i}) \geq 0. \end{cases} \]  

(4.19)

Furthermore, as already explained in section 3.2, the surface integral is approximated by the sum of the fluxes at the integration points of the sub control volume faces multiplied with their respective surface area. Therefore, the effective permeability \( \mathbf{K}_{eff} \) is also evaluated at the integration point, whereas for the hydraulic parameters the upwinding scheme is applied:

\[- \sum_{k=1}^{\text{NoScvf}} \left\{ (\rho_\alpha \frac{k_{ra}}{\mu_\alpha} \mathbf{K}_{eff,ip_k} (\nabla \tilde{p}_{\alpha,ip_k} - \rho_{\alpha,ip_k} \mathbf{g})) \right\}^{t^{+\Delta t}} \cdot \mathbf{n}_k \]

\[- \sum_{k=1}^{\text{NoScvf}} (\phi_{eff} \rho_\alpha \tilde{S}_\alpha)_{upw} \frac{\tilde{u}_t^{+\Delta t} - \tilde{u}_{ip_k}^t}{\Delta t} \cdot \mathbf{n}_k. \]  

(4.20)
4.3 Numerical Models

In the above equation $NoScvf$ is the number of sub control volume faces, $ip_k$ is the integration point on the $k$-th sub control volume face and $n_k$ is its respective unit outer normal vector for the box $B_i$ around node $i$. Transforming the other two terms (see eq. (4.13)) in accordance with equation (3.20) and (3.23), it results the discretized form of the mass balance equations of the $el2p$-model. For all nodes $i$ and phases $\alpha$ it must hold:

$$
V_i \left( \phi_{eff} \rho_\alpha S_\alpha \right)_i^{t+\Delta t} - \left( \phi_{eff} \rho_\alpha S_\alpha \right)_i^t - \sum_{k=1}^{NoScvf} \left\{ \left( \rho_\alpha k_{\alpha \mu} \right)_{upw} K_{eff,ip_k} \left( \nabla \tilde{p}_\alpha,ip_k - \rho_\alpha,ip_k g \right) \right\} \cdot n_k
$$

(4.21)

The terms $\nabla \tilde{p}_\alpha,ip_k, \tilde{u}_k^t$ and $\tilde{u}_k^{t+\Delta t}$ are evaluated at the integration points using the basis functions of the element that contains the respective sub control volume and the respective nodal values.

**Momentum balance equations**

The momentum balance equations (4.15) and (4.12) were discretized with the standard galerkin finite element method, of which the derivation of the respective variational formulation was outlined in section 3.2. However, in the case of the momentum balance equation the unknown is the displacement vector $u$, which is of three dimensions. The introduction of three dimensional test and basis functions is therefore necessary so that each of the unknowns $u_x$, $u_y$ and $u_z$ has appropriate test and basis functions assigned to on each node. On node $i$ there are now existing three $W_{ik}$ and $N_{ik}$, where $k$ denotes the coordinate directions and $k \in \{1,2,3\}$. Equation (4.15) is now multiplied with the introduced test functions and transformed as in section 3.2. Furthermore, for simplification purposes, the matrix $F = \Delta \sigma - \Delta \rho_{el} I$ is introduced:

$$
\int_{\Omega} W_i \cdot \text{div} F \, d\Omega = \int_{\Gamma_{\partial \Omega}} W_i \cdot n \, d\Gamma_{\partial \Omega} - \int_{\Omega} \nabla W_i : F \, d\Omega = 0.
$$

(4.22)

For the sake of simplicity, the neumann boundary condition is set to zero and the equation is reformulated using the index notation. It results the variational form:

$$
\int_{\Omega} W_{ik,j} F_{kj} \, d\Omega = \int_{\Omega} W_{ik,j} \left[ \Delta \sigma_{kj} - \Delta \rho_{el} \delta_{kj} \right] \, d\Omega = 0,
$$

(4.23)

where $\delta_{kj}$ is kronecker’s delta. Note that the Einstein summation convention is used, i.e. it is summed up over indices that occur twice. The three test functions are independent, so when evaluating the equation at node $i$ and coordinate direction $k$, the test functions for the remaining two coordinates of $k$ can be set to zero. Repeating this procedure for the three coordinate directions leads to three equations on each node.
4.4 Coupling concept

The stress tensor $\sigma$ is determined using the linear elastic material law presented in section 2.5.2. The approximations for the primary variables can now be inserted to obtain the discretized formulation. Since the test functions $W_{ik}$ are only non-zero in adjacent elements, the integral over the entire domain can be substituted by the sum over the set of neighboring elements $E_i$. The integration over one element is performed by using a Gauss quadrature rule with $n_G$ points with coordinates $\chi$ and weighting factors $\alpha$. It thus must hold for each test function $W_{ik}$:

$$
\sum_{\chi \in E_i} \sum_{l=1}^{n_G} \alpha_l W_{ik}(\chi_l) [\Delta \sigma_{kj}(\tilde{\mathbf{u}}, \chi_l) - \Delta \rho_{\omega}(\chi_l) \delta_{kj}] = 0, \quad (4.24)
$$

The same procedure can be performed on equation (4.12), leading to:

$$
\sum_{\chi \in E_i} \sum_{l=1}^{n_G} \alpha_l W_{ik}(\chi_l) [\Delta \sigma_{kj}(\tilde{\mathbf{u}}, \chi_l) - \Delta \tilde{p}_{\text{eff}}(\chi_l) \delta_{kj}] \\
+ \sum_{\chi \in E_i} \sum_{l=1}^{n_G} \alpha_l W_{ik}(\chi_l) \left[ \phi_{\text{eff}}(\chi_l) \tilde{S}_n(\chi_l) [\rho_n(\chi_l) - \rho_{\omega}(\chi_l)] \right] g_k = 0. \quad (4.25)
$$

Note that $\tilde{p}_{\text{eff}}$, $\phi_{\text{eff}}$ and the phase densities are also functions of the primary variables (see chapter 2).

4.3.2 Solution Procedure

The solution of the system of the discretized equations presented in the previous section is done fully coupled, that means that the entire system is assembled in one global matrix and solved at once. It has already been mentioned that this approach provides the best description of the feedback of the deformations on the flow processes and vice versa.

Because of the non-linear nature of the mass balance equations, the system is linearized and solved through the application of a Newton-Raphson method (see section 3.4) for each time integration. The solution of the linear system of equation within each Newton iteration is performed using a direct solver called SuperLU (Demmel et al. (1999) [14]), since iterative solvers showed convergence problems for the matrix of the el2p-subdomain (Darcis (2013) [12]).

4.4 Coupling concept

Spatial model coupling is often realized by implementing two adjacent domains and models and defining coupling conditions at their interfaces. This has been done for example in Baber et al. (2011) [1] or Mosthaf et al. (2011) [23]. However, another way is the usage of a volume coupling approach, which can be applied when the different models of the
different subdomains share some of the function spaces. Then it can be suitable to define partially overlapping subdomains, in which the shared function spaces are solved for the whole domain. It is therefore not necessary to define coupling conditions at the interfaces for these function spaces. For the remaining function spaces, which are not shared by all the involved subdomains, boundary conditions have to be defined at the subdomain interfaces.

In this work, the hydro-geomechanical \textit{el2p}-model partially overlaps the geomechanical \textit{el}-model and the two models share the same function spaces for the three displacements $u_x$, $u_y$, $u_z$. The volume coupling is realized within DuMu$^x$ by making use of the DUNE modules Multidomain and Multidomaingrid (Müthing and Bastian (2011) [24]) and the management of the involved function spaces is carried out by the DUNE based general discretization framework PDElab (Bastian et al. (2010) [4]).

Figure 4.2: Illustration of the host grid, two subdomains and the resulting \textit{MultiDomainGrid}

Figure 4.2 depicts the way the volume coupling is realized in the DUNE-Multidomaingrid module. The global grid, or \textit{host grid}, is first transformed into a \textit{MultiDomainGrid}, also called \textit{meta grid}. Now subdomains can be defined randomly on this \textit{meta grid}, that do not have to comprise it entirely. This makes it very easy to adapt the domain size and shape without creating a new host grid.

With respect to the models of this work, only two subdomains have to be defined. The \textit{el}-subdomain can be seen as subdomain 1 and the \textit{el2p}-subdomain as subdomain 2 in figure 4.2. The momentum balance equation of the solid matrix is assembled in the whole simulation domain, i.e. the \textit{el}-domain, but has the form of equation (4.12) in those parts that are overlapped by the \textit{el2p}-domain. In the outer parts equation (4.15) is solved. As already mentioned, due to its assembly in the whole domain, no interface conditions need to be assigned for the three primary variables $u_x$, $u_y$, and $u_z$. For the primary variables $p_w$ and $S_{CO_2}$ of the \textit{el2p}-model, boundary conditions need to be defined at the interface.

4.5 Grid and Boundary Conditions

The Grid used for all the test cases is a radially symmetric grid with an inner radius of 0.05 m, which represents the injection well boundary, and an outer radius of 8000 m (see figure
The domain height is 2000 m and the angle 90°. The reservoir in the model is located at a depth of 990 - 1000 m, which is why the grid is refined in vertical direction around the injection horizon. In horizontal direction the grid is also refined towards the injection well and in angular direction the domain has been discretized with three elements. In total the global grid consists of 7200 hexahedral elements and 10,044 nodes, respectively.

With respect to the geological structure of the model domain, four different layers of rock have been considered. The overburden, between the surface and a depth of 400m, a caprock of 590m thickness, then the aquifer between a depth of 990m and 1km and underneath that 1km of underburden. The respective hydraulic parameters that have been chosen for the different layers are given in table 4.2:

<table>
<thead>
<tr>
<th></th>
<th>underburden</th>
<th>aquifer</th>
<th>caprock</th>
<th>overburden</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability $K$ /m²</td>
<td>$1 \cdot 10^{-19}$</td>
<td>$1.3 \cdot 10^{-14}$</td>
<td>$1 \cdot 10^{-21}$</td>
<td>$1 \cdot 10^{-17}$</td>
</tr>
<tr>
<td>Porosity $\phi$</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>Young’s modulus $E$ /Pa</td>
<td>$2 \cdot 10^{10}$</td>
<td>$6 \cdot 10^{9}$</td>
<td>$2 \cdot 10^{10}$</td>
<td>$1.5 \cdot 10^{9}$</td>
</tr>
<tr>
<td>Poisson’s ratio $\nu$</td>
<td>0.15</td>
<td>0.2</td>
<td>0.15</td>
<td>0.2</td>
</tr>
<tr>
<td>Residual saturations $S_{wr}/S_{nr}$</td>
<td>0.3/0.05</td>
<td>0.3/0.05</td>
<td>0.3/0.05</td>
<td>0.3/0.05</td>
</tr>
<tr>
<td>Entry pressure $p_d$ /Pa</td>
<td>$6.21 \cdot 10^5$</td>
<td>$1.99 \cdot 10^4$</td>
<td>$6.21 \cdot 10^5$</td>
<td>$1.99 \cdot 10^4$</td>
</tr>
<tr>
<td>Brooks-Corey parameter $\lambda_{BC}$</td>
<td>1.078</td>
<td>1.078</td>
<td>1.078</td>
<td>1.078</td>
</tr>
</tbody>
</table>

Table 4.2: Parameters used for the different layers of rock, i.e. the underburden, aquifer, caprock and overburden

In the following the boundary conditions applied in the simulations are presented. Note that for the outer boundary of the el2p-subdomain, i.e. the interface between the two subdomains, the concepts implemented for the boundary conditions are presented in section 4.6 and will not be further discussed here.

**Dirichlet boundaries**

The Dirichlet boundaries are shown in figure 4.3. The dark grey part of the domain indicates the el2p-subdomain and the light grey area the el-subdomain, respectively. On all the lateral boundaries and on the bottom boundary the normal displacements are fixed and set to zero to account for the adjacent masses of rock, which impose a strong resistance on further deformations. These restrictions will have a strong effect on the horizontal displacements within the domain because of the phenomena described in section 4.1. The given Dirichlet boundary conditions thus affect the inner domain on a much larger scale as for example the fluid pressure.

With respect to the mass balances of the two fluids, in the el2p-subdomain, depicted in dark grey, $p_w$ and $S_{CO_2}$ are fixed on the surface. In the case of the reference scenario, i.e an el2p-subdomain size of 8000m, on the outer lateral boundary $p_w$ and $S_{CO_2}$ are also fixed.
Neumann boundary conditions

During the derivation of the variational formulation of the general master balance law in chapter 3, surface integrals over the domain’s Neumann boundary for the flux terms automatically emerged. In the strong formulations of the two problems (see equation 4.13 and 4.16) it could be seen the form of these flux terms. They usually incorporate the derivatives of the primary variables, so what it prescribed on these boundaries is not their values themselves, but more a restriction on how their gradients evolve on it.

With respect to the mass balance equations, it can be seen from the equations, that a mass flux over the boundary can be prescribed. If this mass flux is set to zero, mass transfer over the boundary is prohibited (Neumann no-flow). The momentum balance equation for the solid matrix on the other hand is three dimensional and balances forces, thus on a Neumann boundary it is prescribed a force, which can also be set to zero. In this case the rock experiences no external restrictions on the deformations.

For all the scenarios an injection rate of 0.25 kg/(m$^2$s) has been chosen and imposed as a Neumann boundary condition on the nodes on the inner (well) radius of the aquifer (see figure 4.3). All the other boundaries have been set to Neumann no-flow. With respect to the momentum balance equation, external forces have been set to zero. It has been explained previously, that on the lateral boundaries the normal displacements were fixed in order to model the restrictions the surrounding masses of rock impose on the model domain. However, since the domain extends vertically to the ground surface, a neumann boundary at the ground surface is legitimate since the impact of the above air masses is neglectable.

\[ u_x = u_y = 0 \]
\[ S_{CO_2} = 0, \ p_w = p_{init} \]

\[ u_x = u_y = 0 \]
\[ S_{CO_2} = 0, \ p_w = p_{init} \]

Figure 4.3: The grid used for the simulations and Dirichlet boundary conditions
4.6 Interface boundary conditions

For all the models, a zero saturation boundary condition was chosen for the mass balance of CO$_2$. This arises from the fact that the coupling radius is chosen bigger than the distance the CO$_2$ is travelling in the considered time span. With respect to the mass balance of water, one has to keep in mind that the pressure signal travels much further than the CO$_2$ and thus a flow of water will be observable in far greater distances. Therefore, different approaches for the boundary condition of the mass balance of water have been elaborated.

4.6.1 Approach 1: The Dirichlet model

An intuitive justification for neglecting all fluid flow processes and using a simply mechanical model in the outer domain would be that the chosen coupling radius is bigger than the radius of influence of the injection in the considered time span. In other words, the radius is chosen to be bigger than the distance for which a considerable pressure buildup will occur. The consequence of that is the implementation of a Dirichlet boundary condition for the water pressure in the $el2p$-subdomain at the interface to the $el$-subdomain, where it is set to the initial value. No pressure buildup will occur at the interface and water will flow out of the subdomain.

However, whether a substantial pressure buildup will be observable on the boundary or not, highly depends on the injection rate, the spatial parameters, the simulation time and of course the coupling radius. For a considered time span of simulation this might not be known in advance. It was therefore tried to elaborate more flexible approaches, which are presented below.

4.6.2 Approach 2a: The Theis model

As soon as a considerable pressure buildup occurs on the boundary, the pressure can not further evolve unrestricted if a dirichlet boundary condition is implemented. Therefore, it has been tried to develop an approach, that allows the coupling radius to be smaller than the radius of influence and nevertheless give good results for the pressure distribution. This can only be achieved by accurately modeling the outflow of water out of the $el2p$-subdomain so that the pressure evolves correctly. This task is very difficult and the approaches presented below are rather pragmatic. Also, the water pressure has to be adequately continued in the $el$-subdomain to account for the feedback of the pressure on the rock mechanics. It has therefore been introduced a pseudo pressure $p_{el}$ in the $el$-domain, which is not explicitly calculated in the fully coupled system of equations, but evaluated as a post processing step after each time integration. The obtained pressure distribution in the $el$-domain is then used in the following time step and is therefore time lagged.
The idea behind the following concept is based on the analytical solutions for the drawdown provoked by a steady-state radial flow to a pumping well proposed by Theis (1935) [28]:

\[ s = \frac{Q}{4\pi T} \left[ -\gamma - \ln u - \sum_{n=1}^{\infty} \frac{(-1)^n u^n}{n!} \right], \quad (4.26) \]

where \( u = \frac{r^2 S}{4Tt} \). The derivation and explanation of this equation has been outlined in section 3.6. Due to the assumptions made in the derivation process, the validity of this equation in the given context is certainly not given. However, it is assumed that the curve of the pressure buildup will have a similar shape. For this reason, the two parameters

\[ a = \frac{Q}{4\pi T}, \quad (4.27) \]
\[ b = \frac{4Tt}{S} \quad (4.28) \]

are introduced, which allow for a reformulation of (4.26) to

\[ s = a \left[ -\gamma - \ln \left( \frac{r^2}{b} \right) - \sum_{n=1}^{\infty} \frac{(-1)^n (r^2/b)^n}{n! n (b)^n} \right]. \quad (4.29) \]

As mentioned in section 3.6, the equation has been derived under the assumption of a radially homogeneous and isotropic permeability distribution. Inhomogeneities in radial direction are expected to strongly influence the applicability of this method and have not yet been considered. The main idea of the concept is now to see the pressure distribution in the aquifer as a set of isolated 1D radial pressure curves that connect the nodes on the
well with the radially corresponding nodes on the interface. Figure 4.4 illustrates this idea, however, it is depicted for a node above the aquifer. Note that this is just for illustrative reasons as the grid in the aquifer is very fine.

**Step 1: Curve fitting**

On each of those nodes on the interface, that are within the aquifer, a Gauss-Newton algorithm (see section 3.5) is executed after each time step. This is done to determine parameters $a$ and $b$ for each of those nodes, that best fit equation (4.29) to the actual pressure values on the radially connected nodes towards the injection well. As a result one obtains the before mentioned set of radial pressure curves in the aquifer.

**Step 2: pressure curve reconstruction in the el-subdomain**

As already mentioned above, the consideration of the fluid pressure in the el-subdomain requires the introduction of a pseudo pressure $p_{el}$. With the two parameters at hand for the different nodes on the interface, it is now possible to compute this pressure for the radially connected nodes in the el-subdomain. On each node, $s = \Delta p$ is evaluated using equation (4.29) by inserting its radius and the before calculated parameters, and then added to the inicial pressure value if $\Delta p > 0$. However, since the curves do not exactly match after the fitting, the curve is shifted such that the fitted curve exactly matches the actual pressure value at the node on the interface.

The obtained values for $\Delta p_{el} = \Delta p = p_{el} - p_{init}$ are later introduced in the momentum balance equation of the el-subdomain, equation (4.15). It should be noted that in one timestep, all $\Delta p_{el}$ were evaluated on the previous time level. For big time steps the displacement field in the el-subdomain is therefore expected to show larger discrepancies. The definition of $u$ and thus of the parameter $b$ suggests a linear relation with the time. A parallel model has therefore been elaborated, in which the pressure introduced in the momentum balance equation is not equal to the one calculated in the time step before, but extrapolated in time for the actual timestep size $\Delta t$ calculating a new parameter $b$ in the following way:

$$b_{\text{guess}} = \frac{b}{t} \cdot (t + \Delta t). \quad (4.30)$$

An elaboration of the different approaches is given in section 5.4.

**Step 3: Evaluating the boundary condition**

On all the nodes that incorporate this new approach, the boundary condition for the water pressure is initially set to neumann no-flow and the curve fitting routine is inactive. However, as soon as the model experiences a pressure buildup on these nodes (the threshold value has been defined to 0.5 bar), a curve is fitted to the actual pressure values as described above and the outflow is calculated evaluating the gradient $\nabla s = \nabla p$ of the fitted curve.

\footnote{The author has in mind, that this does not represent the reality, as especially close to the injection well vertical fluxes due to buoyant forces appear. In section 4.6.5 this will be further discussed.}
analytically. This happens on all the considered nodes of the interface independently and after every time step after a pressure buildup was registered. The flux per surface area normal to the subcontrol volume faces that correspond to node $i$ for the next time step is then obtained using Darcy’s Law:

$$F_N = -\frac{\rho_w}{\mu_w} K_{eff} \nabla p.$$  \hfill (4.31)

Note that $K_{eff}$ is a scalar value here because in the model horizontally homogeneous and isotropic permeability layers have been implemented and the calculated outflow is assumed to be in radial direction, which is a direct result of the separation of the aquifer into 1D-radial pressure curves mentioned before. It should also be indicated that the flux $F_N$ corresponds to the flux $F(\tilde{u}) \cdot n$ in the surface integral

$$\int_{\Gamma_{\Omega N}} F(\tilde{u}) \cdot n \ d\Gamma_{\Omega N}$$  \hfill (4.32)

in equation (3.17) for those subcontrol volume faces that are on this neumann boundary.

Note that this concept has only been applied to those nodes on the interface and their corresponding nodes in radial direction (of the el-subdomain), that are within the aquifer. Outside of the aquifer the application of the theis function does not make sense\(^3\). For the remaining nodes on the interface, dirichlet boundary conditions for the water pressure and the CO\(_2\) saturation have been implemented. With respect to the weighting matrix $W$ (see section 3.5), it has been assigned a bigger weighting on the nodes close to the interface in order to reproduce the gradients more accurately.

### 4.6.3 Approach 2b: The Jacob model

In section 3.6 it has been presented a simplification of the Theis equation, found by Jacob and Cooper (1946) \(^{11}\):

$$s = \frac{Q}{4\pi T} \ln \left( \frac{2.25 T t}{r^2 S} \right) \quad \text{for} \quad \frac{r^2 S}{4tT} \leq 0.02.$$  \hfill (4.33)

The restriction $\frac{r^2 S}{4tT} \leq 0.02$ suggests that it is only valid for small radii and/or large times. However, the same idea and algorithm as presented in the section before has also been implemented and tested for equation (3.63) instead of equation 4.26, as by performing a parameter fit only the shape of the equation is important and not its actual applicability.

\(^3\)The author has in mind that the application of the Theis function is also not valid within the aquifer under the conditions prevailing in the models of this work. This has already been mentioned in the beginning of this section.
Again, with the introduction of two parameters
\[
\tilde{a} = \frac{Q}{4\pi T}, \quad (4.34)
\]
\[
\tilde{b} = \frac{2.25 T t}{S}, \quad (4.35)
\]
this equation can also be rewritten into a parametrized form:
\[
s = \tilde{a} \ln \left( \frac{\tilde{b} r^2}{\tilde{a}} \right). \quad (4.36)
\]

The same steps as in the model presented in the previous section can now be performed. However, the simpler form of equation (4.36) allows for another way of making the fitted curve match exactly to the actual pressure value on the interface. It is done using the following equation, which is a simple transformation of equation (4.36) inserting the values at the interface. Instead of shifting the curve as in the Theis model, the parameter $b$ is changed in order for the curves to match.
\[
\tilde{b}_{\text{new}} = \exp\left( \frac{\Delta p_{\text{interface}}}{\tilde{a}} \right) \cdot (r_{\text{interface}})^2. \quad (4.37)
\]

This guarantees that the curve is continuous at the interface. For the Jacob model a parallel model including an extrapolated pressure distribution in time has also been implemented. The concept has been introduced in the previous section. This extrapolation is also done using equation (4.30), as the two parameters show the same correlation with the time.

For both the Jacob and the Theis model, the outflux depends on the values of the old time step. It is thus expected that the introduced error depends on the time step size. An evaluation of this can be found in section 5.4.

### 4.6.4 Approach 3: The moving model

When looking at the problem as it is described in the introduction of this chapter another idea for the coupling of the two models emerges intuitively. In the early stages after the injection has started, an important pressure increase will only be observable in areas close to the injection well, while in the rest of the domain the pressure stays on its initial value. Thus, the idea comes up to increase the el2p-subdomain with time depending on the actual pressure distribution. The model should recognize the need of an enlargement of the el2p-subdomain early enough in order for the boundary condition to not affect the pressure evolution in the inner domain. The interface boundary condition in this case is set to Dirichlet assigning the initial pressure value to the respective nodes.
For the development of an algorithm that detects the need of an enlargement of the el2p-subdomain, it has been looked at equation (3.63) and especially at the definition of the radius of influence. In this context, the radius of influence is defined as:

\[ R = \sqrt{\frac{2.25 T t}{S}}. \] (4.38)

When defining \( \tilde{r} := \frac{2.25 T}{S} \), the equation can be reformulated to:

\[ R = \sqrt{\tilde{r} t} \] (4.39)

and the following inequality is valid:

\[ R(t + \Delta t) = \sqrt{\tilde{r}(t + \Delta t)} < \sqrt{\tilde{r} t + \sqrt{\tilde{r} \Delta t}} = R(t) + \sqrt{\tilde{r} \Delta t}. \] (4.40)

Note that \( \tilde{r} \) only depends on aquifer and fluid parameters and can therefore be estimated and is not depending on the primary variables. Using equation (4.40), it can now be calculated an underestimate of the Radius \( R(t) \), which has to be already passed by the pressure signal in order for it to reach the el2p-subdomain boundary, i.e the interface, for the next time step size \( \Delta t \):

\[ R(t) = r_{\text{interface}} - \sqrt{\tilde{r} \Delta t}. \] (4.41)

If, after a time integration, the model detects a pressure buildup bigger than a threshold value (here: 0.2 bar) for radii bigger than the calculated radius \( R(t) \), the subdomain is resized using a new radius calculated by the following formula:

\[ R_{\text{new}} = r_{\text{interface}} + \sqrt{\tilde{r} \Delta t}. \] (4.42)

This is again an overestimate, so it is expected that the model not only detects the need of an enlargement of the el2p-subdomain early enough, but that the amplification of the subdomain size is also big enough to not have to resize after every time step. A detailed evaluation of the model’s behaviour is found in section 5.5.

As explained in section 4.4, the el2p-subdomain is overlapping the el-subdomain and the latter exists on the whole grid. Therefore, values for the primary variables of the el-model are at hand for the whole domain. Furthermore, the initial pressure distribution of the el2p-model is continued in the el-model before starting the simulation. When increasing the el2p-subdomain size, values for the primary variables have to be assigned to the added nodes. Since these nodes previously were already part of the el-domain, the values for the displacements can be copied to the solution of the new el2p-subdomain after creating it.
Moreover, the two remaining primary variables $p_w$ and $S_{CO_2}$ have to be set. As a natural consequence of the concept behind this model it is assigned $p = p_{init}$ and $S_{CO_2} = 0$ for the newly created nodes.

### 4.6.5 Remarks

The approaches presented in the sections 4.6.2 and 4.6.3 aim for the reconstruction of the pressure information in the $el$-subdomain based on the information in the $el2p$-subdomain and for the modeling of the flux that would occur at the interface if it was not there. With the latter, it is tried to achieve a correct evolution of the pressure within the $el2p$-subdomain. The author has in mind that the chosen approach does not provide an elaborate mathematical derivation and that it is of a more pragmatic nature. Different and less pragmatic approaches for the modeling of the outflux had been tried but led to convergence problems and thus no usable results. With respect to the pressure extrapolation, it has been already stated that the author is aware of the fact that the chosen analytical solutions involved in these two models are not applicable for the actual problem in their original formulation. A more formal way of deriving the mutual interaction between the subdomains would be the study of the influx in the outer domain caused by a unit pressure increase at the inner boundary. This would lead to a response function for the pressure, which can be used in the model by saving the pressure increases appearing on the boundary over time and then reconstruct the outflow into the outer domain via convolution.

Since for this response no analytical solution is available and it is furthermore not trivial to derive, it could be evaluated numerically by modeling only the outer domain imposing a unit pressure increase as boundary condition where the interface would be. The result for the step function depends on different parameters, as for example the chosen permeability of the aquifer, and a large study with the evaluation of numerous simulations would be necessary in order to generalize the response function for the development of a flexible and adjustable model. And even by doing this, it remains questionable if a usable relationship can be found. Because of it’s simpleness and relatively easy implementation, the in sections 4.6.2 and 4.6.3 presented approaches have nevertheless been implemented and tested. With respect to the moving model presented in section 4.6.4 it should also be noted that it lacks a formal mathematical derivation and is again rather pragmatic.
Chapter 5

Results

For the determination of the performance of the different approaches, simulations have been realized for various coupling radii and compared to a model of full complexity, i.e. the simulation of the whole domain with the el2p-model. The comparison was done with respect to the speed-up achieved by the coupling and the introduced error, respectively. An injection time of 5 years has been simulated on the grid presented in 4.5 using the mechanical and hydraulic parameters from table 4.5. Note that the subsequent plots, when referred to as plots through the aquifer, were obtained by evaluating the nodes at a depth of 993.76m (in the middle of the aquifer) and an angle of 30°. Figure 5.1 gives an illustration of the path that was used for this evaluation.

Figure 5.1: Illustration of the path that was used for the evaluation of the plots through the aquifer

For an easier understanding of the subsequent sections, the figure on the following page gives a graphical overview over the simulations that were performed and should be used during the lecture of this chapter.
Figure 5.2: Graphical overview over the performed simulations. The blue areas depict the el2p and the grey areas the el-subdomain. The indicated lengths denote the radial distance from the injection well. Indicated are the scenarios that were performed on the different grid partitions and the respective boundary condition type.
5.1 The Dirichlet model

The implementation of a Dirichlet boundary condition at the outer boundary of the \textit{el2p}-subdomain is assumed to have a big effect on the pressure evolution within the aquifer depending on the time scales that are aimed to be modeled. As soon as a considerable pressure buildup would be observable on the interface, the dirichlet boundary condition leads to an outflow of fluid and the pressure at the interface stays on a fixed value. Thus, with time the error in the pressure distribution increases and also leads to errors in the displacement field since it is driven by the pressure. In this section, simulations have been performed for varying coupling radii, while the overall size of the model domain stayed constant. This series of simulations is motivated by the fact, that one does not know in advance whether or not the chosen coupling radius will influence the pressure evolution within the domain for the considered time span and the chosen hydraulic parameters. The findings of these simulations could give an idea of how much this eventually wrong pressure affects the results.

The radii were chosen to 2000, 4000 and 6000m and the respective simulations will from now on be referred to as R2, R4 and R6. Table 5.1 shows the numbers of global degrees of freedom for the different coupling scenarios.

<table>
<thead>
<tr>
<th>coupling radius /m</th>
<th>2000</th>
<th>4000</th>
<th>6000</th>
<th>8000</th>
</tr>
</thead>
<tbody>
<tr>
<td>degrees of freedom</td>
<td>46,500</td>
<td>48,484</td>
<td>49,476</td>
<td>50,220</td>
</tr>
</tbody>
</table>

Table 5.1: Number of degrees of freedom for the different coupling scenarios

A big reduction in the number of degrees of freedom can not be achieved because only two out of the five primary variables are neglected in the outer subdomain and furthermore the grid is refined towards the injection well, leaving most of the nodes within the \textit{el2p}-subdomain. The refinement chosen for the aquifer is also existent in the \textit{el}-subdomain, which further limits the reachable reduction of degrees of freedom. Since the grid has a maximum radius of 8000 m (see section 4.5), this is chosen as the reference simulation (R8).

5.1.1 Error introduced by the coupling

In the following, the deviations in the simulation results for the different coupling scenarios are demonstrated for the primary variables and the spatial parameters $\phi_{\text{eff}}$ and $K_{\text{eff}}$. These errors are first quantified and presented in a descriptive manner in the sequel before discussed and interpreted in the last section.
5.1 The Dirichlet model

Pressure evolution

Figure 5.3 shows the pressure evolution in the aquifer for different simulation times and coupling radii.

As expected, the pressure is underestimated after a significant buildup has reached the el2p-boundary and the error increases with time. The maximum absolute and their corresponding relative deviations with respect to R8 for the plot are listed in table 5.2. Furthermore, it is shown the euclidian norm of the error:

\[ ||e||_2 = \sqrt{\sum_{i=1}^{\text{noNodes}} (p_{\text{scenario},i} - p_{R8,i})^2}. \]  

(5.1)

As it can be seen from the plots, the maximum deviations occur on the nodes that are
located on the interface and they result smaller for increasing coupling radii. The euclidian norm of the error shows the same decline (see table 5.3).

<table>
<thead>
<tr>
<th>coupling radius /m</th>
<th>2000</th>
<th>4000</th>
<th>6000</th>
</tr>
</thead>
<tbody>
<tr>
<td>max absolute deviation /bar</td>
<td>9.877</td>
<td>3.014</td>
<td>0.969</td>
</tr>
<tr>
<td>corresponding relative deviation /%</td>
<td>8.5791</td>
<td>2.7839</td>
<td>0.9122</td>
</tr>
<tr>
<td>radius of occurrence /m</td>
<td>2007.5</td>
<td>4200.4</td>
<td>6074.2</td>
</tr>
<tr>
<td>euclidian norm $</td>
<td></td>
<td>e</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.2: Maximum pressure deviations in the aquifer with respect to R8 for the different coupling radii at $t = 5y$.

With respect to the maximum occurring pressure, i.e. the pressure at the well, the relative errors are very small for all the different simulations. As depicted in figure 5.4, the pressure reaches its peak value within the first months of the simulation time and it is identically reproduced by the different coupling scenarios. The error then increases with time and reaches a value of 4.6% for the R2, 0.6% for the R4 and 0.05% for R6 relative to the R8.

![Figure 5.4: Pressure at the well over the simulation time](image)

Solid displacements

Because of the strong coupling between the pressure and the displacements of the solid matrix, the results of the latter are expected to reflect the above shown deviations in the pressure evolution. In figure 5.5, the displacements $u_x$ and $u_z$ within the aquifer for different simulation times are plotted over the radius. The obtained curves for $u_y$ are of identical shape as those for $u_x$, for which reason they are not further illustrated here. A comparison of figure 5.5a and 5.3a looking at the results for R8, shows that after one year of injection
displacements occur in distances to the well where a noticeable pressure buildup can still not be observed, which substantiates the preliminary motivation for the model coupling given in section 4.1. This especially holds for the horizontal displacements, as they have Dirichlet boundary conditions assigned to on the interface. This can be confirmed by the plots for $u_z$ in figure 5.5, for which a Neumann boundary condition has been applied and which follow more or less the pressure evolution. Significant vertical displacements can not be observed in distances much further than the extent of the pressure signal.

Figure 5.5: Solid displacements within the aquifer for different simulation times

The peak value of the horizontal displacements, at a radius of approximately 200m, is reproduced well for all the scenarios, whereas large discrepancies are observable between R2 and R8 for radii bigger than 500m and a simulation time of $t = 5$ years. The error seems to be significantly reduced when the radius is doubled from 2km to 4km. This statement is supported by the values for the maximum errors in plot 5.5c and 5.5d which are shown
5.1 The Dirichlet model

in table 5.3. Doubling the coupling radius from 2km to 4km led to a quartering of the maximum absolute deviation.

<table>
<thead>
<tr>
<th>coupling radius /m</th>
<th>2000</th>
<th>4000</th>
<th>6000</th>
</tr>
</thead>
<tbody>
<tr>
<td>max absolute deviation $u_x/(m \cdot 10^{-4})$</td>
<td>2.10</td>
<td>0.42</td>
<td>0.20</td>
</tr>
<tr>
<td>radius of occurrence /m</td>
<td>2904.2</td>
<td>5051.2</td>
<td>5539.2</td>
</tr>
<tr>
<td>euclidian norm $|e|_2/(m \cdot 10^{-4})$</td>
<td>7.13</td>
<td>0.97</td>
<td>0.65</td>
</tr>
<tr>
<td>max absolute deviation $u_z/(m \cdot 10^{-3})$</td>
<td>1.20</td>
<td>0.36</td>
<td>0.12</td>
</tr>
<tr>
<td>radius of occurrence /m</td>
<td>1830.4</td>
<td>4200.4</td>
<td>6074.2</td>
</tr>
<tr>
<td>euclidian norm $|e|_2/(m \cdot 10^{-3})$</td>
<td>9.10</td>
<td>1.60</td>
<td>0.32</td>
</tr>
</tbody>
</table>

Table 5.3: Maximum deviations for $u_x$ and $u_z$ in the aquifer with respect to R8 for the different coupling radii at $t = 5y$.

In figure 5.6, the surface uplift above the well is depicted over the simulation time for the node at the surface above the well and at an angle of 30°. As for the pressure, the deviations are reduced significantly when doubling the radius from 2km to 4km. The relative deviations result in 39.61% for the R2, 7.10% for R4 and 1.28% for R6 and are thus a bit higher than for the pressure at the well.

![Figure 5.6: Surface uplift at the well over the simulation time](image)

**Spatial parameters**

The relations between the pressure, the displacements and their feedback on the spatial parameters has been illustrated in section 2.1. Summing up, the pressure buildup leads to displacements which then lead to an increase in porosity and permeability, which in turn has an impact on the flow field. The plots for the spatial parameters $\phi_{eff}$ and $K_{eff}$ in the
5.1 The Dirichlet model

The curves for the final simulation time of 5 years reflect this correlation, as the curves have almost identical shape to the ones obtained for the pressure (see figure 5.7).

\[ \text{Figure 5.7: radial effective porosity (a) and permeability (b) distribution at the final simulation time of } t = 5y \]

\textbf{Saturation distribution}

In figure 5.8 the radial saturation distribution in the aquifer at the final simulation time of 5 years is depict. It can be seen that for all the different coupling radii the CO\textsubscript{2} travels only until a distance of approximately 450 m in the considered time span, which legitimates the implemented interface boundary condition of $S_{CO_2} = 0$. The saturation front is reproduced very well in R4 and R6 with a maximum absolute deviation of 0.0071 (relative deviation: 13.05%) and 0.002 (3.76%), both appearing at a radius of 415.33 m. With respect to R2, the error is a bit bigger with a maximum absolute deviation of 0.0632 (116.2%).

\[ \text{Figure 5.8: Radial saturation distribution in the aquifer at } t = 5y \]
5.1 The Dirichlet model

Summary and discussion

The results shown in the above sections reproduced the behaviour that was expected previously and led to errors of different dimensions for the different considered quantities. It should be mentioned that the deviations presented in the above tables were evaluated for the shown plots, however, the values correspond to the maximum deviations found in the whole simulation domain, which is why they were not presented separately. It was seen that, depending on the considered time scale, this coupling concept leads to errors in the pressure evolution or more precisely in an underestimate of the pressure and larger radial pressure gradients (see figure 5.3). The maximum presented relative errors for the final simulation time were below 10% and appeared on the interfaces. Moreover, the smaller pressures in the aquifer led to smaller vertical displacements \( u_z \) in the aquifer were of very similar shape to those obtained for the pressure. That is because for \( u_z \) both on the inner and the outer vertical boundary, as well as on the top of the reservoir, Neumann boundary conditions were applied, which allows the rock to relax on the boundaries in terms of stresses. The surface uplift above the well was, like the pressure buildup, reproduced well for coupling radii bigger than 4km, leading to relative errors below 10 % (see figure 5.6). For the horizontal displacements different effects could be observed. First of all, the influence of the boundaries is noticeable, since the gradients of the horizontal displacements towards the boundary are relatively steep\(^1\). In the R2 scenario they were underestimated, which can again be explained by the smaller pressure. With respect to R4 and R6 though, the differences in pressure are not that drastic and a light overestimation of \( u_x \) (and \( u_y \)) within the inner domain, i.e the el2p-subdomain, could be observed. This can be explained by the larger pressure gradients in radial direction in comparison to R8, which exert a radial force on the rock matrix. The decrease in pressure is thus compensated and even lightly overcompensated so that the displacements are slightly larger than those occurring for R8 in that region. For radii larger than the coupling radius, the displacements are underestimated though, which is due to the fact that at these distances there is neither a pressure increase nor a pressure gradient observable, since a purely mechanical model is solved and a fluid is not considered.

With respect to the saturation front, it has been seen that for the smaller coupling radii

\(^1\)A model without boundary effects on the inner displacement field is almost impossible though, since the domain would have to be chosen extremely large.
5.1 The Dirichlet model

the saturation front is a bit steeper and seems to travel a bit further (figure 5.8). This might again be explained by the larger pressure gradients for smaller coupling radii, leading to higher flow velocities. In other words, a smaller body of water bearing less resistance to the propagation of the saturation front, is modeled.

The errors in pressure for later simulation times were already expected in advance. However, no noticeable deviations occurred until a significant pressure buildup actually reached the interface. This could lead to the assumption, that the solid displacements were reproduced good enough for an adequate modeling of their feedback on the rock’s hydraulic parameters. But it could also be a result of the fact that the biggest errors were observable in terms of the horizontal displacements, however, these are comparatively than the vertical displacements, which is a natural consequence of the boundary condition at the surface. Their influence on the calculation of the effective porosity and permeability is thus smaller. This is substantiated by the plots in figure 5.7. It thus remains open, if the better calculation of the displacements, by enlarging the domain where the mechanics are included, led to the observed good reproduction of the pressure in the early simulation stages, or if the effect is just very small. If so, the mechanical domain would not have to be enlarged in order to accurately model the pressure evolution. This will be investigated in section 5.2.

5.1.2 Speed-up due to coupling

It is now looked at the performance of the different scenarios with respect to the computational cost. For the study of the speed-up achieved by the coupling it is examined the CPU time, the average assembly time of the global matrix and the average linear solver time for the Newton iterations.

CPU time

Figure 5.9 shows the different CPU times plotted over the model time. It is noticeable that an increasing speed-up for decreasing radii, as it was expected, can not be observed at the final simulation time. For small simulation times under one year the curves align in the expected order, however, at a model time of approximately 1.1 years, the slope of the curve for R2 increases. The curves for the R4 and the R6 scenario keep evolving similarly until at \( t \approx 3.2 \) years the one for R4 also shows a kink and the CPU times tend to higher values.

A shape as it was expected can only be seen on the curve for the R6 scenario. The R8 curve shows abrupt slope changes as well, which indicates bad convergence behaviour and will be discussed later. Against the expectations, it can now be observed an increasing speedup for increasing radii, however, the R8 scenario was computationally most expensive. The speedup achieved was 10.7% for the R2, 15.2% for the R4 and 24.1% for R6. But it should be kept in mind that for model times below 3 years, all the coupled scenarios led to substantial speed-ups.
5.1 The Dirichlet model

Assembly and linear solver time

The assembly time for the global matrix depends on the number of degrees of freedom and is expected to be reduced when reducing the \( e2p \)-subdomain size. The same is valid for the linear solver time, as a smaller global matrix should be solved faster. These parameters are independent from the convergence behaviour and thus more reliable parameters for the quantification of the speed-up introduced by the coupling. In figure 5.10 they are depicted for the different coupling radii and show the behaviour as anticipated. The speedup for the average assembly time can be quantified to 17.1% for R2, 8.2% and 2.1% for R4 and R6, respectively. With respect to the average linear solver time, the observed speedups were 24.9%, 19.00% and 12.9% for the radii in increasing order.

Figure 5.10: Average assembly (a) and linear solver time (b) for the different coupling radii
5.1 The Dirichlet model

Number of time steps

The study of the number of time steps needed for the simulation is crucial for the interpretation and comparison of the CPU times presented in the first section, as the time step size is a direct consequence of the convergence behaviour of the Newton solver. A larger number of time steps in a given period thus hints at small time step sizes and a rather poor convergence of the solver.

![Graph showing number of time steps](image)

Figure 5.11: Number of time steps needed for the different years of the simulation time

Figure 5.11 shows the number of time steps needed by the different scenarios for the different years of the simulation time. Since the simulation is started with an initially small time step of 1\( s \), it is natural that in the first year more time steps are required. Also, right after the start of the injection there are initially strong gradients, which lead to a worse convergence behaviour and therefore the time step size might not be increased as fast. Over the time the time steps get larger according to the convergence of the Newton solver, which can be observed in figure 5.11. R4 and R6 seem to show the best convergence behaviour, which can be seen in the faster decrease of the number of time steps. However, R4 shows an increase of the time step sizes again in the fourth year of the simulation. The same holds for R2 in the fifth year. For the sake of completeness, in table 5.4 there are listed the total numbers of timesteps that were required for the different simulations.

<table>
<thead>
<tr>
<th>coupling radius /m</th>
<th>2000</th>
<th>4000</th>
<th>6000</th>
<th>8000</th>
</tr>
</thead>
<tbody>
<tr>
<td>number of time steps</td>
<td>223</td>
<td>195</td>
<td>168</td>
<td>230</td>
</tr>
</tbody>
</table>

Table 5.4: Total number of timesteps required for the different coupling scenarios
Summary and discussion
The speedup with respect to the CPU time for the whole simulation showed the opposite
behaviour to the one that was expected. The observed speedup increased for increasing
coupling radii (figure 5.9) even though the average assembly and linear solver times were
reduced (figure 5.10). This can be explained by the number of time steps that were nec-
essary for the simulation, caused by a bad convergence behaviour for smaller coupling radii
at later simulation times. One could try to explain this with the steeper pressure gradients
in the el2p-subdomain caused by the imposed Dirichlet boundary condition. In R4 these
develop at later times which could explain the kink at \( t \approx 3.2 \) years. On the other hand,
this disagrees with the worse convergence of R8 in comparison to R6, as well as it could
not describe the kink for R2 at \( t \approx 4 \) years. Thus, the approach for an explanation remains
speculation. R6 showed a speed up of 24.1\%, which is mainly due to the lower number of
time steps required for the simulation. It is still not clear why the convergence follows this
rather random behaviour.

Depending on the time scale of interest, a speed-up could be achieved through the applica-
tion of spatial model coupling. The assembly and linear solver times confirm this speedup,
however, its significance is questionable due to the convergence issues. The assembly is
realized faster, because less degrees of freedom are considered resulting in a smaller ma-
trix, which again leads to faster linear solver times. The concave shape of the relation
between the average assembly time and the coupling radius (figure 5.10a) can be explained
by differences in the number of degrees of freedom between the different coupling scenarios.
Increasing the radius from 2km to 4km led to an increase in degrees of freedom of 1984
additional unknowns, whereas from R4 to R6 only 992 and from R6 to R8 only 744 degrees
of freedom were added. An explanation for the convex shape of the curve in figure 5.10b
could not yet be found.

5.2 The Dirichlet model - revisited

In the precedent sections, the R8 scenario has been used as a reference to which the results
of the coupled models were compared. It was seen that the error between the coupled mod-
els and R8 depend on the considered time scales and on the regarded quantities. Before
an important pressure buildup was observable on the interface between the subdomains,
the pressure was reproduced identically. As already mentioned, this could be explained by
a correct reproduction of the aquifer’s hydraulic parameters as a result of the calculation
of the displacement field in the whole model domain. However, looking at the scale of the
increase in permeability in figure 5.7b the effect is assumed to be neglectable. Furth-
more, the vertical displacements are of one order of magnitude bigger than the horizontal
displacements, their influence on the calculation of the effective permeability is thus bigger.
On top of that, because of the Neumann boundary imposed on the top boundary, \( u_z \) is
highly correlated to the pressure and evolves less influenced by the outer lateral boundary. It
is thus expected that a larger mechanical domain is not necessary for a correct reproduction of the pressure.

Nevertheless, if the focus is on the mechanical quantities, e.g. for risk estimations and the evaluation of failure conditions, the enlargement of the mechanical subdomain might be required. Both questions are addressed in the following sections.

5.2.1 Hydraulic considerations

It was said that the feedback of the mechanics on the flow field is expected to be neglectable. For the determination of this question, three more simulations are introduced in this section. The simulations of only the el2p-subdomains from R2 and R4 will from now on be referred to as the el2p2000 and el2p4000 scenario. On top of that, a grid with a maximum radius of 20km has been created and simulated applying the el2p-model in an inner domain with a radius of 8km. This simulation (from now on referred to as the DispR20 scenario) is used for a comparison to R8.

The results revealed that the pressure distributions between the non-coupled models and the models with an enlarged geomechanical subdomain do not show noticeable deviations. The pressure seems to evolve identically, as figure 5.12 depicts.

![Figure 5.12: A comparison of the pressure in the aquifer between R2 (a) and R4 (b) with their respective non coupled models, i.e. el2p2000 and el2p4000.](image)

Shown are the comparisons of R2 and R4 with the respective non-coupled models. The results for R8 in comparison with DispR20 are not explicitly shown here, as the outcome is the same. As already mentioned, the influence of the horizontal displacements on the hydraulic parameters of the aquifer is estimated to be relatively small in comparison to the vertical displacements. These were shown to be highly correlated to the pressure, for what reason the spatial parameter distribution is expected to be very similar for the coupled
and non-coupled models. Figure 5.13 shows the effective permeability through the aquifer for R2 in comparison with the el2p2000 scenario. No noticeable deviations are observable, which confirms the above mentioned expectations. On top of that, the influence of this increase is assumed to be marginal, since its maximum value (at the well) corresponds to a change in permeability below 4%. The hydraulic quantities seem to be reproduced identical and unaffected by an enlargement of the geomechanical subdomain.

![Effective permeability distribution through the aquifer for R2 in comparison with the el2p2000 scenario](image)

Figure 5.13: Effective permeability distribution through the aquifer for R2 in comparison with the el2p2000 scenario

5.2.2 Mechanical considerations

The horizontal displacements are expected to show deviations caused by the boundary effects of the outer lateral boundary. Figure 5.14 shows the comparisons between R4 and el2p4000 and R8 and DispR20, respectively. As already stated in the previous section, boundary effects originating from the outer lateral boundary are assumed to be nearly impossible to avoid.

The plots in figure 5.14 substantiate this assumption, as the two curves above show a very similar shape, only on different spatial scales. This similarity can also be expressed in numbers. When calculating the ratio between the deviation of the two curves at the interface, i.e. the outer lateral boundary of the non coupled models, and the maximum value for $u_x$ occurring in the coupled model for both of the plots, it is obtained 0.58 for the left and 0.56 for the right plot$^2$. The absolute deviations on the interface are $2.49 \times 10^{-4}$ and $2.40 \times 10^{-4}$. These similarities lead to the assumption that the effects caused by the

$^2$If the maximum radius of the elastic-subdomain of the DispR20 scenario had been chosen to be 16km, these values are expected to be even closer together as the ratio of the subdomain sizes would be the same in that case.
outer Dirichlet boundary do not depend on the absolute sizes of the two subdomains, but only on their ratio. This indicates that the regarded domain sizes are far from being sufficiently big for the boundary effects to decline.

![Graph](a)  ![Graph](b)

Figure 5.14: A comparison of $u_x$ in the aquifer between R4 (a) and R8 (b) with their respective non coupled models, i.e. el2p4000 and DispR20.

With respect to the vertical displacements $u_z$, the results for the coupled and the non-coupled models show rather small deviations. They originate from the fact, that for the non-coupled models, the Neumann boundary condition allows greater deformations in that region as in the coupled case, where the resistance against deformation by the surrounding rock masses is taken into account. However, it was seen in the previous section that the vertical displacements more or less follow the pressure, which is almost identical (see figure 5.12). Therefore the deviations result in rather small values, as figure 5.15 indicates.

![Graph](R8_DispR20)

Figure 5.15: Vertical displacement field in the aquifer for R8 in comparison with DispR20
Assuming the errors in the horizontal displacements are unavoidable, it remains open whether a more accurate reproduction is necessary for the calculation of parameters of interest with respect to rock failure. It has been seen that for the pressure evolution the size of the mechanical subdomain did not matter, as the horizontal displacements did not seem to have a big influence on the calculation of the hydraulic parameters (and the change of permeability is very small). However, the calculation of critical pressure values for tensile and shear failure is correlated to the principal stresses which in turn are related to the displacements. For the fundamentals with respect to their determination, it is referred to Darcis (2013) [12]. The evaluation of the two critical pressure values and a comparison between the coupled and non-coupled models, showed that even for the purpose of identifying eventual shear or tensile failure, an enlargement of the mechanical subdomain did not affect the results. This could be different in non-homogeneous geological layers though.

5.3 Interpretation and comment

The analyzation of the simulation results for the Dirichlet model showed, that calculating the displacement field on a larger scale did not affect the pressure evolution, nor did it influence the calculation of critical pressures with respect to rock failure. That means that the spatial model coupling as presented in this work, is not necessary for the determination of quantities of e.g. political interest. Moreover, the achievable speed-up is questionable because of the presented convergence issues. However, as stated above, this has been evaluated for an idealized system of radially homogeneous geological layers and it might be different if heterogeneous or anisotropic rock is considered. In Darcis (2013) [12], the coupling was realized in the opposite way. A hydro-geomechanical model was solved in the inner domain closer to the injection well, while the aquifer was extended horizontally and a two-phase flow model was applied to this extension. Therefore, boundary conditions for the solid displacements had to be assigned at the boundary of the inner sub-domain, which then highly influenced the displacement field and thus led to differences in the spatial parameters for different coupling radii. As a result, the pressure was overestimated for small coupling radii (Darcis (2013) [12]).

Combining this fact with the observations made in the previous sections, the change in the hydraulic rock parameters due to the displacements actually has a considerable impact on the pressure evolution, but again, it seems obsolete to calculate them on a larger spatial scale. The approach of choosing the inner subdomain, which includes the mechanics, to be smaller than the hydromechanical subdomain is not legitimate from a physical point of view. However, with respect to certain quantities, better results than with the model presented in this work can be achieved. In the following figure 5.16 the R2 scenarios for the two opposite ways of performing the coupling are again compared to R8 (which is identical for both coupling methods). It can be seen that both the pressure above the well, as well as the surface uplift was reproduced better in Darcis (2013) [12].
5.4 The Theis/Jacob model

For a better approximation of the pressure field in the aquifer, even after a prominent pressure buildup has reached the interface, the outflow of water out of the \( \text{el2p}\)-subdomain has to be adequately modeled. If the pressure can be reproduced better than with the application of a Dirichlet boundary condition, the displacements, especially \( u_z \), are also expected to be modeled more accurately.
The idea behind this model was presented in the sections 4.6.2 and 4.6.3. The author is aware of the fact that this approach is very pragmatic and it is not claimed that perfect results can be achieved. However, it is hoped that a certain time span after a Dirichlet boundary would lead to noticeable errors, can be modeled decently. Since there is no regulative algorithm included in the approach, the system is expected to diverge after a certain number of time steps due to error propagation. Furthermore, it is considered the fact that this approach can only be applied to simple horizontally layered geological systems and thus might not be applicable to real problems. It could be reformulated for non-horizontal layers, but the inclusion of heterogeneities within the aquifer is considered to be impossible. On top of that, it is essential that the coupling radius is substantially bigger than the two phase flow region close to the injection well.

It was already mentioned that the equation proposed by Jacob and Cooper (1946) \[11\] (equation (3.63)) represents an approximation of the Theis equation (3.61) for small radii and/or large times. Its form is a lot simpler though and the fitting algorithm, which is the main feature of these models, is expected to be a lot faster than for the Theis equation. With respect to the Theis equation, the infinite series has been truncated after the fifth element, which is often used as a rule of thumb by hydrologists. For the testing of the two models, simulations for coupling radii of 2000m and 4000m have been performed for both of the equations. The results are presented in the following and are again compared to R8 and furthermore to the respective simulation with the Dirichlet model.

### 5.4.1 Coupling radius of 2000m

The corresponding simulations to the coupling radius of 2000m will from now be referred to as the Jacob2000 and the Theis2000 scenario. The comparison is done with respect to R8 and R2 in order to estimate the error introduced by the concept.

**Pressure**

The pressure, representing the driving force for the whole system, is the key quantity of which the accurate modeling should be addressed primarily. Figure 5.17 shows the pressure in the aquifer for different simulation times. The fitting routine was called for the first time, i.e. a pressure buildup of 0.5bar was detected, at a model time of \(t = 0.17\) years. The first plot, figure 5.17a shows the pressure shortly after that, at \(t = 0.2\) years. It can be seen, that the fluxes calculated from the curves fitted to the actual pressure distributions generally are an underestimate, as for later times the pressure increases too much for the Theis/Jacob model. The application of these fluxes on the interface boundary causes a too rapid increase of the pressure at the interface, which leads to smaller gradients in that region. In the subsequent time steps curves are fitted to these less steep pressure distributions which in turn lead to a smaller calculated outflux. The system thus diverges, as there is no stabilizing routine included in the code. A prediction of unphysical pressure evolutions towards too high pressures is not trivial though and it could not yet be found.
5.4 The Theis/Jacob model

such a formulation.

However, until $t = 0.6$ years, the deviations of the pressure at the interface are rather small. Moreover, the curve for the Jacob model is more or less identical to the one for R8 which is hard to see from the plot. 28 timesteps were performed between the first call of the fitting routine and a model time of 0.6 years, which indicates that the outflux initially was modeled decently. It could also be due to the still relatively small time steps, which will be picked up in the subsequent section. The outflux seemed to be modeled very similarly for the Theis and the Jacob equation, which can be seen from the very small differences in the pressure distribution within the inner $el2p$-subdomain. The extrapolation into the $el$-subdomain though led to different pressures for large radii.

A look at the temporal evolution of the pressure suggests that initially the gradient and thus the outflux was well approximated and underestimated for larger times. The question
now is, if the fitted curves do not reproduce well the gradient at the interface, or if it is just due to the before mentioned error propagation. Figure 5.18 shows the actual pressure buildup in the aquifer and the fitted curves for the Theis (curves on the left side) and the Jacob equation (curves on the right side).

Figure 5.18: Actual pressure buildup in comparison to the fitted curves for the Jacob equation (a and c) and the Theis equation (b and d) at different model times

They are shown for $t = 0.4$ and $0.8$ years. It can be seen that the quality of the fits does not differ substantially for the two equations. On top of that, when comparing the gradients of the fits to the gradient of the actual curve towards the interface, it cannot be identified a noticeable underestimation of it for $t = 0.8$ years. The gradient seems to be similarly well reproduced for both of the considered time steps. However, small deviations might be sufficient for the system to diverge. It could also be possible that the error originates from the fact that the gradients are evaluated based on the results of the previous time
step, as in reality the outflux would not be constant but would increase with time. Further
statements on this will be given in section 5.4.3. In any case, it should be noted that for
small time spans after the pressure buildup reached the interface, this model led to better
results for the pressure than the Dirichlet model (see figure 5.17).

Solid displacements
For a model time of \( t = 0.6 \) years, it was seen that the pressure curves for the Theis/Jacob
models were very similar to the one for R8. This should be reflected in the solid displacement
distribution, which is given in figure 5.19. It can easily be recognized that the displacements
were modeled more accurately than with the respective simulation with the Dirichlet model,
which especially holds for \( u_x \). A discussion and possible explanation of the kink that appears
at the interface for \( u_x \) will be given in the following section.

![Solid displacements](image)

Figure 5.19: Solid displacements \( u_x \) (a) and \( u_z \) (b) in the aquifer at \( t = 0.6 \) years, shown
for the Theis/Jacob model as well as R2 and R8

5.4.2 Coupling radius of 4000m
For a coupling radius of 4000m, the model showed a behaviour similar to what was described
in the above. The pressure was modeled well for a certain time span after the buildup had
reached the interface. However, for a radius of 4000m, the algorithm is activated at a later
model time and thus for larger time step sizes. Nevertheless, after the first time the fitting
routine was called (at \( t = 0.9y \)), 36 time steps were performed until the system started
diverging (at \( t \approx 2.8y \)), thus even more as for the coupling radius of 2000m. Moreover,
the extent of the deviations and the speed with which they are evolving are a lot smaller.

Pressure
The above mentioned smaller deviations can be seen in the plots in figure 5.20. Longer
time scales could be modeled without introducing huge errors, however, for later simulation
times ($t > 3$ years) the system does diverge. The quality of the fits was similar to the ones depicted in the previous section and did not vary considerably throughout the simulation. For $t = 2.7$ years, the pressure curves for the Theis/Jacob model conform well to the one for R8, for what reason the displacement fields are later discussed for that timestep.

![Graphs showing pressure changes over time](image)

Figure 5.20: Pressure in the aquifer for different simulation times

Figure 5.21 gives a detailed view on the pressure curves around the interface radius, in order to allow for a possible explanation of the displacement field in that region, which will be discussed in the sequel.
Solid displacements

Before the Jacob/Theis model started diverging, the vertical displacements \( u_z \) were again calculated better than with the Dirichlet model (R4). When looking at the plots in figure 5.22, i.e. for a model time of \( t = 2.7 \) years, it is noticeable that the horizontal displacements exhibit two kinks and a rather unexpected behaviour in the region around the \( el2p \)-boundary.

In the region behind the \( el2p \)-subdomain boundary, \( u_x \) is reproduced better with the Theis/Jacob model than with the Dirichlet model, which can be attributed to the extrapolated pressure. Close to the boundary the curves deviate more though, which could be explained by the larger deviations between the pressure curves in that region (see figure
5.21 But even though the deviations in pressure are bigger for the Jacob model, the Theis model produced slightly larger deviations with respect to $u_x$, which could invalidate this argumentation. However, the differences between the Jacob and the Theis model are very small and could be due to small differences in other parts of the domain.

5.4.3 Remarks

Note that the in section 4.6.2 and 4.6.3 presented concepts for the temporal extrapolation of the pressure introduced in the momentum balance equation of the $el$-subdomain, has not been discussed. This is because for the time scales on which the model still produced decent results, the temporal extrapolation did not have any considerable effect due to the still relatively small time step sizes. The approach could be an improving feature of the model with respect to large time step sizes, however, this is currently obsolete as the results obtained by the model would have to be improved first. This has to be achieved by modeling the outflow at the boundary of the $el2p$-subdomain more precisely.

Furthermore, no information on computational cost or an eventual speed-up was given. This is due to the fact that the fitting algorithm is still computationally very expensive, which originates from the way it is implemented. There is a huge potential on reducing this computational cost, which is why it does not make sense to discuss a possible speed-up at the moment.

The big problem of this model is that the flux is not modeled accurately, which leads to the observed overestimated pressure increase. It should be stated again, that the author was aware of this divergence problem already before implementing this concept. The main focus of this concept was on the effect the extrapolation of the pressure has on the mechanical response of the outer domain and if it leads to improved results in the displacement field. But, in order to be able to study its applicability, the outflux has to be well posed. However, it was expected and it was seen that on a small time scale decent results could be produced which allow for a study of the mentioned effects. It was seen that the extrapolation of the pressure into the $el$-subdomain led to improvements in the reproduction of the displacement field, which justifies its application. But, generally the modeling of the outflux in the way it was done in the above is inappropriate. Other ways of implementing the neumann boundary condition have been tried, however, problems with respect to the convergence of the newton solver were encountered and could not yet be solved.

Furthermore, it should be mentioned that the curve fits were quite poor. The Theis and Jacob equation do not seem to be appropriate functions for the fitting. Fitting the actual pressure values to another function with more parameters could lead to way better fits and eventually a better extrapolation of the pressure. It would not fix the problems with respect to the boundary condition. A more physical, numerically stabilizing and less pragmatic solution to this has to be found.
5.5 The moving model

In section 5.1, it was seen that a large number of time integrations was performed within the first year of the model time. That is a result of the small initial time step size, which is then rather slowly increased in the beginning until the initially steep gradients have leveled out. The R6 scenario showed good convergence over the whole simulation time, indicated by a monotonous evolution of the time step sizes. For this simulation, 21.4% of the time steps originated from the first 3.65 days of the simulation time and 26% from the first 1.2 months, respectively. These numbers highlight the impact of the simulation’s early stages on the computational time. A further characteristic of these early stages is the limited spatial extent where an important pressure buildup can be observed. It is thus expected a big potential on saving CPU time by restricting the calculation of the two phase flow processes to those parts of the domain where they are dominant and by increasing the subdomain size according to the pressure within it. For this reason, the model has been initialized with a coupling radius of 50m, which then subsequently was increased according to the in section 4.6.1 presented idea and algorithm.

The introduced parameter $\tilde{r} = \frac{2.25 T}{S}$ represents something like the “velocity” with which the pressure signal is traveling radially. It depends on the rock parameters $T$ and $S$, whereupon the storage coefficient $S$ can only be guessed for the chosen rock type. Furthermore, the expression for $\tilde{r}$ corresponds to an analytic solution which can only be applied under certain idealizing assumptions. It is thus not known whether the “velocity” will be well approximated or under- or overestimated. However, the expression used for the determination of the necessity for an enlargement of the $el2p$-subdomain, equation 4.41, was an overestimate. In case the pressure increases a bit faster than anticipated by $\tilde{r}$, the algorithm might compensate this circumstance and still produce good results. In the opposite case, the results will be unaffected, only the performance is not maximized with respect to the speed-up. The analyzation of the results therefore focusses, amongst other things, on the accuracy with which the front of the pressure signal is estimated.

For the chosen permeability of the aquifer and an assumed value of $S = 2 \cdot 10^{-5}$, it resulted $\tilde{r}_0 = 1.36$, which will from now on be called the base case. The respective results will be outlined and discussed in the sequel.

5.5.1 The base case

Error introduced by the concept

In the following the results obtained with this model are again compared to R8, the reference scenario (see section 5.1), by drawing a comparison between the results of the two models at the final simulation time of 5 years. The results produced by this model are identical to the reference scenario, only tiny deviations are observable for the horizontal displacements. With respect to the pressure distribution, this is illustrated in figure 5.23.
The maximum deviation of the two curves depicted in the figure above is $4 \cdot 10^{-3}$ bar which corresponds to a relative error of 0.0028 % and therefore is neglectable. The same conclusion can be drawn when regarding the displacements, as shown in figure 5.24. The horizontal displacements seem to be slightly overestimated, however, the maximum deviation, occurring at a radius of 3830 m, and is only $4.78 \cdot 10^{-6} \text{ m} \equiv 1.7\%$.

**Performance of the algorithm**

As seen in the above, no noticeable errors were introduced in comparison to the R8 scenario. The question now is, how often and how much the domain was increased in order to determine if the potential on the speed up has been exploited.
As figure 5.25 depicts, the domain had to be resized 14 times until the coupling radius reached the outer boundary and the whole domain was simulated with the el2p-model, i.e. the full complex model. Furthermore, this has been reached after 1.4 years of simulation time. When looking at the pressure distributions after one and two years of model time (figures 5.3a and 5.3b), one can identify tiny pressure deviations between the R6 and the R8 scenario, suggesting that the pressure has indeed been influenced by the outer boundary in this time frame. However, these deviations are very small and are expected to be neglectable. The algorithm thus seems to handle the resizing in an overcautious manner, i.e. detecting the necessity for an enlargement too early. This can also be seen when looking at the pressure distributions for which a resizing was executed together with its further evolution (figure 5.26).

In figure 5.26a it is depict the pressure in the aquifer for which the first resizing is performed, i.e. an enlargement of the coupling radius, from 50m to 75m. It shows that a considerable buildup has traveled up to a radius of approximately 20m and thus the boundary at 50m still had not affected its evolution. But, the pressure did not reach the radius of 50m until three time steps later (red dotted line), and the buildup furthermore is very small on the respective node. The effect is shown as well in figure 5.26b, where is depict the pressure for the increasing of the coupling radius from 2400m to 3500m. It is observable that neither the pressure had been traveled close to the subdomain boundary of 2400m (black dotted line), nor did it in the subsequent time step (red dotted line). The algorithm thus overestimates the “velocity” with which the pressure is traveling. For this reason further simulations have been realized for $\tilde{r}_1 = 0.7 \tilde{r}_0$, in order to see if similarly good results can be reproduced even for a less cautious algorithm (see section 5.5.2).
5.5 The moving model

Despite the overestimation of the distance the pressure is traveling within one time step, a substantial speed up could be achieved by the method. The speed-up for the whole simulation was 19\% and in the time frame until the last resizing, i.e. in the first 1.4 years, a speed up of 26.25\% was achieved (see figure 5.27a). The speed up naturally declines with increasing model times, as the influence of the speed up achieved within the first 1.4 years decreases.

For the entire simulation 229 time steps were necessary, so the speed up in comparison to R8 can be directly related to the assembly and linear solver time, as differences in the convergence behaviour could not be observed. Of these 229 time steps, 126 have been

Figure 5.26: Two exemplary pressure distributions for which the domain was resized, the black dotted line is the radius before resizing

Figure 5.27: CPU time vs. model time (a) and speed-up vs. model time (b)
performed within the first 1.4 years and furthermore half of the latter were performed with a radius of 6660.82m (see figure 5.28a). A less cautious handling of the \textit{el2p}-subdomain size is thus expected to hold further potential on a possible speed-up.

Figure 5.28b shows the assembly and the linear solver time plotted over the simulation time until the final resizing. One can identify the times where a resizing is performed in an increase of both of these parameters. Furthermore, this increase becomes smaller as the radii become larger, which is due to the fact that the grid is refined towards the injection well. It can also be observed that substantially faster assembly and linear solver times only occurred on a very small temporal scale in the beginning of the simulation. However, it has already been mentioned the importance of this period on the overall computational cost.

![Figure 5.28: Number of time steps vs. model time (a) and assembly/linear solver time vs. model time (b). The red dots in (a) indicate the times where a resizing was performed.](image)

The times that were necessary for the resizing are depicted in figure 5.29. With increasing radius the required time increases up to a value of 306s, which is in the dimension of one time step. In total, resizing the grid 14 times took 2902.1s, which is neglectably small in comparison to the CPU time for the whole simulation.

![Figure 5.29: Times necessary for the resizing of the \textit{el2p}-subdomain](image)
5.5 The moving model

Summary and discussion

It has been seen that a substantial speed up could be achieved by the method while reproducing the results of the fully complex model. For the used value of $\tilde{r}_0 = 1.36$, the propagation of the pressure seemed to have been overestimated and thus the enlargement of the subdomain according to equation 4.42 was overestimated as well. As mentioned, half of the time steps until the final resizing were already performed with a radius of 6660.82m, which leaves potential on a further speed up if the condition for the enlargement of the subdomain is adjusted to a less cautious one. It is thus expected that it can be further increased by adjusting $\tilde{r}$ while still obtaining good results. An investigation of this is given in the subsequent section.

Big differences in the convergence behaviour could not be construed from the plot in figure 5.27a, in any case though, the average assembly and linear solver time of the global matrix are more reliable parameters and are listed in table 5.5. Considerable differences in these parameters can be found, which verifies the significance of the previously stated speed-up.

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<th>moving model</th>
<th>R8</th>
<th>speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>assembly time (t &lt; 1.4y)</td>
<td>110s</td>
<td>139s</td>
<td>21%</td>
</tr>
<tr>
<td>assembly time (whole simulation)</td>
<td>122s</td>
<td>139s</td>
<td>12%</td>
</tr>
<tr>
<td>lin. solver time (t &lt; 1.4y)</td>
<td>49s</td>
<td>78s</td>
<td>37%</td>
</tr>
<tr>
<td>lin. solver time (whole simulation)</td>
<td>53s</td>
<td>75s</td>
<td>29%</td>
</tr>
</tbody>
</table>

Table 5.5: Average assembly and linear solver time in comparison to R8, evaluated for the first 1.4 years (until the final resizing step) and for the whole simulation time

5.5.2 Modified propagation velocity

The above presented way of determining the need for an enlargement of the $el2p$-subdomain is overcautious, i.e. the subdomain size increases earlier than necessary. This could be due to the fact that the chosen inequality (4.41) for the estimation of the distance a significant pressure buildup is propagating in one time step, is already an overestimate. Furthermore it is questionable if the idealized equation (3.63) is a good representation of the pressure propagation in this particular case. The results produced by the base case were already quite pleasant, however, it is expected that there is more available potential on saving computational time. It has therefore been introduced a factor, with which the parameter $\tilde{r}$ is multiplied in order to adapt the propagation “velocity” suggested by equation 3.63. Another simulation has been performed with $\tilde{r}_1 = 0.7 \tilde{r}_0$, of which the results are presented in the following

Introduced error

The smaller value for $\tilde{r}$ did not affect the results of the simulation. The results are identically to the base case, which is why they are not further presented here, but it is instead focussed
on the effects on the computational cost.

**Speed-up**

A look at the CPU times reveals, that for $\tilde{r}_1 = 0.7 \tilde{r}_0$, the speed-up with respect to the base case could be further increased substantially (see figure 5.30).

![Figure 5.30: A comparison of the CPU times for the two values of $\tilde{r}$](image)

The convergence behaviour for this new simulation seemed to be different from the two others, however, a comparison with figure 5.9 shows that the curve has a similar shape to the one for R6 for simulation times below 4.4 years. For that reason these two simulations are now further compared, but, it should be kept in mind that the R6 scenario did not reproduce the results of R8 perfectly. The worse convergence behaviour of R8 could not yet be explained.

![Figure 5.31: The $\tilde{r}_1$ scenario in comparison to R6 with respect to the CPU time (a) and the achieved speed-up (b).](image)

The two indicated points in (b) are the time for which the last resizing is done (left) and the speed-up for $t = 4$ years, before the convergence behaviour of the $\tilde{r}_1$ scenario worsens.
It is legitimate to assume that if R8 converged well, showing a similar behaviour to R6, the CPU time would be higher in comparison to R6 and thus the speed up achieved by the moving model even bigger. Nevertheless, as figure 5.31 shows, a significant speed-up could be achieved.

A look into the log-file of the simulation of the $\tilde{r}_1$ scenario shows, that at $t = 4.4$ years the newton solver does not converge in one time step. The time step size is then reduced drastically, which is the reason why the slope changes temporarily. However, figure 5.31b reveals that a considerable speed-up could be achieved for $t < 4$ years between 20-25%. With respect to the R8 scenario it is in the range of 40-45%, but this can not be directly compared due to the differing convergence behaviour of the simulations. Therefore, the average matrix assembly and linear solver times are listed in table 5.6.

<table>
<thead>
<tr>
<th>Time Interval</th>
<th>R8</th>
<th>Base case</th>
<th>$\tilde{r}_1$ scenario</th>
</tr>
</thead>
<tbody>
<tr>
<td>Assembly time (t &lt; 1.8y) /s</td>
<td>139</td>
<td>113</td>
<td>101</td>
</tr>
<tr>
<td>Speed-up with respect to R8 /%</td>
<td>-</td>
<td>18.7</td>
<td>27.3</td>
</tr>
<tr>
<td>Assembly time (whole simulation) /s</td>
<td>139</td>
<td>122</td>
<td>117</td>
</tr>
<tr>
<td>Speed-up with respect to R8 /%</td>
<td>-</td>
<td>12.2</td>
<td>15.8</td>
</tr>
<tr>
<td>Linear solver time (t &lt; 1.8y) /s</td>
<td>78</td>
<td>50</td>
<td>51</td>
</tr>
<tr>
<td>Speed-up with respect to R8 /%</td>
<td>-</td>
<td>35.9</td>
<td>34.6</td>
</tr>
<tr>
<td>Lin. solver time (whole simulation) /s</td>
<td>75</td>
<td>53</td>
<td>54</td>
</tr>
<tr>
<td>Speed-up with respect to R8 /%</td>
<td>-</td>
<td>29.3</td>
<td>28</td>
</tr>
</tbody>
</table>

Table 5.6: Average assembly and linear solver time in comparison to R8, evaluated for the first 1.8 years (until the final resizing step of the $\tilde{r}_1$ scenario) and for the whole simulation time.

It is noticeable, that the average assembly time of the global matrix could be further reduced, but in contrast to that the linear solver time showed a slight increase. An explanation for this could not yet be found. Due to the different magnitudes though, an overall speedup is expected. Especially for the first 1.8 years of the simulation, the speed-up achieved by the $\tilde{r}_1$ scenario is a lot bigger, almost twice as high. The coupling radii were smaller in the early stages of the simulation (see figure 5.32), which should have a relatively big influence because of the mentioned high number of time steps in the beginning of the simulations and the refinement of the grid towards the injection well.
Figure 5.32: Coupling radii plotted over time for the two values of $\tilde{r}$
Chapter 6

Summary and outlook

In this work, spatially coupled models for the simulation of CO₂ sequestration in deep saline aquifers have been presented. The coupling was realized by a volume coupling approach that was explained in section 4.4. For the treatment of the appearing interface, three different approaches were implemented and tested and led to different results.

It was seen that by applying a Dirichlet boundary condition at the outer boundary of the inner el2p-subdomain, the model produces results that agree well with those of a full complex model in the early stages of the simulation (see section 5.1), while leading to a speed-up in comparison to the reference scenario. However, for later simulation times, errors with respect to the pressure occur as a natural consequence of the chosen boundary condition. Furthermore, convergence problems emerged, leading to larger computation times and a reduction of the achievable speed-up. The obtainable speed-up is also limited due to the fact that the refinement of the grid within the aquifer extends to the el-subdomain. Since in this region a linear elastic material law is used, i.e. the descriptive set of equations is linear, a fine grid is unnecessary. The speed-up is thus expected to be a lot larger when performing the coupling by defining two separate subdomains, coupling conditions on the interface and two grids of different refinements. This would require a model that is able to handle “hanging nodes” on the coupling interface. The coupling in the presented way has the advantage that the coupling radius can be adjusted very easily without having to create a new grid. However, it was seen that whether or not the application of the coupling makes sense thus strongly depends on the time scales that are sought to be modeled and, as also seen in section 5.1, the quantities of interest. The comparison between the coupled and non-coupled scenarios in section 5.2 showed that the calculation of the displacement field on a larger scale than the flow processes did not affect the pressure evolution within the el2p-subdomain, nor did it change the outcome with respect to the critical pressures for shear or tensile failure. The spatial coupling might thus be obsolete, but, in case of radially heterogeneous layers with fragile rock in greater distances to the injection well, the presented coupling could be a useful tool.

It was furthermore seen that the correct modeling of the pressure is crucial for the whole system, as it is its driving force. With the Theis/Jacob model presented in section 5.4, it
was tried to diminish the errors introduced by the Dirichlet model for later simulation times, i.e. the errors in the pressure evolution. However, the system started diverging relatively fast because of the chosen implementation of the outflow boundary condition at the outer boundary of the $el2p$-subdomain. The author is aware of the fact that this boundary condition is not mathematically founded and inappropriate. Finding a correct outflow condition is not trivial and the ones that were elaborated prior to the presented one led to convergence problems and thus no usable results. Therefore it was chosen in the presented way in order to be able to study the system’s response to the extrapolated pressure. It could be observed that the extrapolation of the pressure led to improvements in the calculation of the displacement field before the system started diverging. Moreover, the curve fits were quite poor, which leads to the assumption that the choice of a more adequate and flexible function could improve the results substantially. This would not solve the problem of the outflow boundary though, which is why the finding of an adequate boundary condition would be the most important goal of future works. However, the approach is only applicable to idealized problems with a certain geometry and is thus not flexible. It is therefore questionable if it makes sense to elaborate further improvements on this model, as its relevance might not be given in the context of real problems.

The moving model presented in section 5.5 is able to adjust the $el2p$-subdomain size depending on the actual pressure distribution and identically reproduced the results of the reference scenario. Furthermore, a substantial speed-up could be achieved by the method in the range of 20-25%. The “propagation velocity” of the pressure signal chosen for the determination of the necessity to enlarge the subdomain, is based on an analytical solution that is not applicable for the regarded problem (see section 4.6.4). It was seen that this “velocity” was overestimated, thus the speedup could be further increased by finding a more appropriate formulation. It could also be possible, that similarly good results could be obtained by choosing a Neumann no-flow boundary and increasing the subdomain after a buildup was observable. Future work could adress these two issues. But it should be noted that this method is also not general and only applicable to horizontally layered aquifers. For a further generalization it should be modified such that the algorithm can handle non horizontal layers and inhomogeneities in horizontal direction.
Bibliography


Appendix A

Consider a random motion of an arbitrary body $B$ as illustrated in figure A.1. The configuration $B_0$ is called referential configuration and is a constant reference with respect to which the motion is described. The coordinates $X$ denote material points of the referential and $x$ are the coordinates of the actual configuration. The motion of the material points can be expressed by a bijective motion function

$$x = \chi(X, t).$$  \hspace{1cm} (A.1)

The bijectivity of $\chi$ claims the existence of an inverse motion function $X = \chi^{-1}(x, t)$ and therefore a non-singular Jacobian:

$$\det J = \det \frac{\partial x}{\partial X} \neq 0.$$  \hspace{1cm} (A.2)
Under these considerations the material deformation gradient $F = \frac{\partial x}{\partial X}$ can be introduced and the following transformations can be derived:

\begin{align*}
    &dx = F dX \quad \text{(A.3)} \\
    &da = (\det F) F^{-T} dA \quad \text{(A.4)} \\
    &dv = (\det F) dV, \quad \text{(A.5)}
\end{align*}

with $dx$ and $dX$ being material line elements, $da$ and $dA$ surface elements and $dv$ and $dV$ volume elements of the referential and the actual configuration. The time derivative $\dot{d\Omega}$ from chapter 2.3 can now be expressed with respect to the constant referential configuration as

\[d\dot{\Omega} = [ (\det F) d\Omega_0 ] = (\det F) d\Omega_0, \quad \text{(A.6)}\]

where the transformation A.5 has been used and the subscript 0 denotes the initial state, i.e. the referential configuration. Performing the time derivative in index notation and using the chain rule of differentiation, it can be shown that $\det F = (\text{div } v) F$, with the displacement velocity $v = \frac{\partial u}{\partial t}$. This results in the following relation:

\[d\dot{\Omega} = (\det F) d\Omega_0 = (\text{div } v) F d\Omega_0 = (\text{div } v) d\Omega. \quad \text{(A.7)}\]
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