Solution strategies for nonlinear conservation laws

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Abstract

Nonlinear conservation laws form the basis for models for a wide range of physical phenomena. Finding an optimal strategy for solving these problems can be challenging, and a good strategy for one problem may fail spectacularly for others. As different problems have different challenging features, exploiting knowledge about the problem structure is a key factor in achieving an efficient solution strategy.

Most strategies found in literature for solving nonlinear problems involve a linearization step, usually using Newton's method, which replaces the original nonlinear problem by an iteration process consisting of a series of linear problems. A large effort is then spent on finding a good strategy for solving these linear problems. This involves choosing suitable preconditioners and linear solvers. This approach is in many cases a good choice and a multitude of different methods have been developed.

However, the linearization step to some degree involves a loss of information about the original problem. This is not necessarily critical, but in many cases the structure of the nonlinear problem can be exploited to a larger extent than what is possible when working solely on the linearized problem. This may involve knowledge about dominating physical processes and specifically on whether a process is near equilibrium.

By using nonlinear preconditioning techniques developed in recent years, certain attractive features such as automatic localization of computations to parts of the problem domain with the highest degree of nonlinearities arise. In the present work, these methods are further refined to obtain a framework for nonlinear preconditioning that also takes into account equilibrium information. This framework is developed mainly in the context of porous media, but in a general manner, allowing for application to a wide range of problems. A scalability study shows that the method is scalable for challenging two-phase flow problems. It is also demonstrated for nonlinear elasticity problems.

Some models arising from nonlinear conservation laws are best solved using completely different strategies than the approach outlined above. One such example can be found in the field of surface gravity waves. For special types of nonlinear waves, such as solitary waves and undular bores, the well-known Korteweg-de Vries (KdV) equation has been shown to be a suitable model. This equation has many interesting properties not typical of nonlinear equations which may be exploited in the solver, and strategies usually reserved to linear problems may be applied. In this work includes a comparative study of two discretization methods with highly different properties for this equation.

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List of publications

Paper A: Skogestad, J.O. & Kalisch, H. (2009): "*A boundary value problem for the KdV equation: Comparison of finite-difference and Chebyshev methods*", Mathematics and Computers in Simulation, Vol 80 (1), pages 151-163.

Paper B: Skogestad, J.O.; Keilegavlen, E. & Nordbotten, J.M. (2013): "*Domain decomposition strategies for nonlinear flow problems in porous media*", Journal of Computational Physics, Vol 234, Pages 439-451.

Paper C: Skogestad, J.O.; Keilegavlen, E. & Nordbotten, J.M. (2015): "*Two-scale Preconditioning for Two-phase Nonlinear Flows in Porous Media*". Preprint, submitted to Transport in Porous Media.

Paper D: Keilegavlen, E.; Skogestad, J.O. & Nordbotten, J.M. (2014): "*Domain decomposition preconditioning for non-linear elasticity problems*", Proceedings of 11th World Congress of Computational Mechanics, Barcelona.

Contents

Part I: Background

1. Introduction

The desire to understand the forces of nature has followed the human civilization since its inception, not primarily for the sake of the understanding itself, but rather for survival, either by taming the forces or by learning how to adapt to or avoid them. As science and mathematics has progressed, these forces and the large variety of related natural phenomena have been described by physical laws. Among the most fundamental of these laws are the conservation laws, which state that certain properties in a system cannot simply appear or disappear, but change at a rate balancing the rate of net flux between the system and the surroundings. In classical mechanics, conservation laws for mass, energy, momentum and angular momentum form the basis for a multitude of other physical laws, which may be derived from, or turn out as special cases of these.

With the relativity theories by Einstein in the early 20^{th} century, the classical Newtonian laws were found not to be universally valid. In this new view, with mass and energy equivalent and time depending on the reference frame, new and adjusted conservation laws were needed. However, this applies first and foremost to phenomena at sub-atomic or astronomic scales, and does not invalidate the classical models for intermediate scales. The phenomena considered in this work are well within the domain of classical mechanics, so relativity is not needed and thus not considered here.

Still, the interesting length and time scales span several orders of magnitude, from flow through tiny pores in a rock to global scale weather systems and ocean circulation patterns, and from fractions of a second to millions of years. Although the conservation laws are scale independent, by incorporating phenomena at all relevant scales, performing practical calculations that produce valid results on all scales is challenging.

The nonlinear nature of the phenomena described poses another practical challenge. Linear problems represent a special case for which solution strategies are more easily

devised than for most nonlinear problems. A rich literature of mathematical solution strategies for different kinds of linear problems exists, many of which are applicable to a broad range of problems. Nonlinear problems, on the other hand, are generally much harder to solve. In fact, the most common solution strategies consist of converting the problem to a sequence of linear problems through an iterative method.

The key to a successful strategy for a given nonlinear problem, lies in identifying characteristic features that may be exploited in the solvers. In this work, we will look into a few selected areas with different challenges related to nonlinear conservation laws, and identify suitable strategies for each.

In the case of surface gravity waves on water, it may not come as a surprise that complex phenomena such as wave breaking, freak waves and undular bores call for a nonlinear description. But also very simple wave forms such as a single solitary wave travelling along a canal have a nonlinear nature. The Korteweg de Vries (KdV) equation provides a model for certain nonlinear waves that we will look into here.

Flows in porous media such as oil reservoirs and groundwater aquifers also generally behave strongly nonlinearly, with nonlinearities arising various relations between different properties, such as relative permeabilities for different fluid phases, capillary pressure relations and nonlinear couplings between different governing equations. Heterogeneous parameter fields and a great span in relevant length and time scales further complicates the situation.

Elasticity is an important property of solid materials and is important to consider in a large variety of applications, e.g. in construction projects and in studies of swaying trees. The relation between applied stress and strain may be strongly nonlinear and calls for a nonlinear solution strategy.

With these three physical application areas as a starting point, we will present different nonlinear models and solution strategies. In particular, we will try to devise strategies that challenge the standard procedure of linearizing first and then applying specialized methods such as preconditioning and advanced linear solvers, by working

directly on the original nonlinear problem. With methods developed in recent years, it is more viable to take such an approach now than just a couple of decades ago.

2. Conservation laws in physical systems

Conservation laws are among the most fundamental building blocks for models of physical phenomena. This chapter presents conservation laws in general form, and discusses a few common formulations, before moving on to some of the fundamental special cases of conservation laws, namely conservation of mass, momentum and energy.

2.1 General conservation laws and different formulations

Conservation of mass, energy, momentum, angular momentum and electrical charge are the fundamental principles in classical physics [118,142]. Conservation laws may also be defined for derived properties. In this work we will focus on conservation of mass and momentum, and models derived from these. We also briefly present energy conservation.

Conservation of a property means that in an isolated system, the property does not change with time. By allowing sources and sinks and open boundaries, balance laws, which state that the net change of the property equals the net amount of the property entering and leaving the domain, and continuity equations can be formed. Continuity equations have the additional property of local conservation, in the sense that transport of the conserved quantity must be continuous. In this work we follow the convention of letting the term 'conservation law' also cover these equations.

Figure 2.1 illustrates the concept of conservation of a property, whose density is χ, for an arbitrary isolated system, represented by the domain Ω. The boundary of the domain is denoted by $\partial\Omega$ and the outward unit normal vector on $\partial\Omega$ is $\vec{n}$. Conservation laws form the link between the laws of nature and a mathematical model by ensuring that fundamental principles are obeyed in the model, e.g. that energy cannot be created or vanish or that mass cannot simply appear or disappear, but must come from somewhere. Model equations derived from conservation laws may have entirely different characteristics from each other, depending on the physical

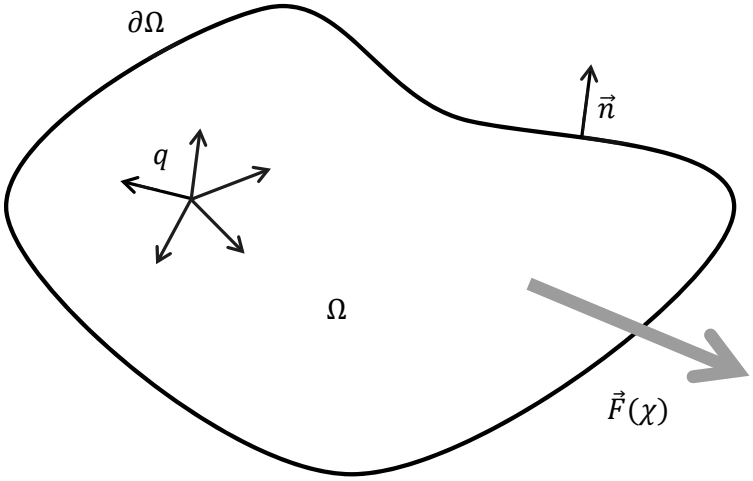

Figure 2.1: Conservation of a property χ in a volume Ω with a point source q and outflux $\vec{F}(\chi)$ across the boundary $\partial\Omega$ with outer unit normal vector $\vec{n}$.

phenomena they are set to model. When devising a solution strategy, this is crucial to consider. Hence, the choice of solution method depends heavily on the characteristics of the problem, and for different solution methods different formulations of the problem may be desirable. A few common formulations of a general conservation law as described above will be presented briefly in the following paragraphs. For a more comprehensive introduction, see e.g. [3,4,118,142].

2.1.1 Integral formulation

In mathematical terms, the rate of change of property χ in Ω, which is assumed to be fixed in space, is

$$\int_{\Omega} \frac{\partial \chi}{\partial t}\, dV\,. \tag{2.1}$$

The outward flux of χ across $\partial\Omega$ is

$$\int_{\partial\Omega} \vec{F}(\chi) \cdot \vec{n}\, dS. \tag{2.2}$$

The integral form of the conservation law is obtained by combining equations (2.1) and (2.2) and introducing the source term q, which integrated over Ω represents the net influx of χ through sources and sinks within the domain:

$$\frac{d}{dt}\int_{\Omega} \chi \, dV + \int_{\partial\Omega} \vec{F}(\chi) \cdot \vec{n} \, dS - \int_{\Omega} q \, dV = 0. \tag{2.3}$$

This equation states that the accumulation over time of χ in Ω balances with the net contribution from flow across the $\partial\Omega$ and sources and sinks within the domain.

2.1.2 Differential formulation

Using Gauss' divergence theorem on equation (2.2) yields an alternative formulation of the flux integral, assuming that $\vec{F}(\chi)$ is continuously differentiable,

$$\int_{\partial\Omega} \vec{F}(\chi) \cdot \vec{n} \, dS = \int_{\Omega} \nabla \cdot \vec{F}(\chi) dV. \tag{2.4}$$

Substituting this in equation (2.3) gives

$$\int_{\Omega} \left(\frac{\partial \chi}{\partial t} + \nabla \cdot \vec{F}(\chi) - q \right) dV = 0. \tag{2.5}$$

Since this equation is to hold for any Ω, the integrand must be zero and the integral sign can be removed to yield the partial differential equation

$$\frac{\partial \chi}{\partial t} + \nabla \cdot \vec{F}(\chi) = q, \tag{2.6}$$

which is the differential formulation of the general conservation law.

2.1.3 Weak formulation

Sometimes it is useful to formulate the conservation law as a minimization problem. This can be done by casting the problem on weak form, where 'weak' refers to the fact that the requirements of smoothness of the functions are weaker when the problem is posed on this form. We will for simplicity consider this for a case where the time

derivative term vanishes, i.e. the system is in steady-state. Further, if the flux $\vec{F}$ can be expressed in terms of a potential, say $\vec{F}(\chi) = a(x)\nabla\xi$, the problem can be stated as

$$\nabla \cdot a(x)\nabla\xi = q. \tag{2.7}$$

In this presentation, homogeneous Dirichlet conditions on $\partial\Omega$ are assumed, but the presentation is readily extendable to general boundary conditions [4]. Let $\mathcal{H}_0^1(\Omega)$ be the Sobolev space of L^2-continuous functions with compact support in Ω and L^2-continuous first order derivatives. By multiplying equation (2.7) with a function $\zeta \in \mathcal{H}_0^1(\Omega)$ and integrating over Ω, we obtain the weak form of the conservation law:

$$\int_\Omega \nabla\zeta^T a(x)\nabla\xi \, dV = \int_\Omega q^T\zeta \, dV . \tag{2.8}$$

The problem then consists of finding ξ such that equation (2.8) holds for all $\zeta \in \mathcal{H}_0^1(\Omega)$ [4]. Equation (2.8) may be expressed in terms of a bilinear form and an inner product,

$$b(\zeta, \xi) = (q, \zeta) \tag{2.9}$$

where the bilinear form $b(\,,)$ is defined as

$$b(u, v) = \int_\Omega \nabla u^T a(x)\nabla v \, dV, \tag{2.10}$$

and $(\,,)$ denotes the standard L^2 inner product on Ω,

$$(u, v) = \int_\Omega u^T v \, dV, \tag{2.11}$$

In the case of $a(x) \equiv I$, where I is the identity operator, $b(u, v)$ reduces to $(\nabla u, \nabla v)$.

2.2 Some fundamental conservation laws

In this section we will outline some specific conservation laws that are fundamental to modelling of physical phenomena. Specifically, conservation of mass and momentum is considered, followed by a brief presentation of conservation of energy. The differential form presented in Section 2.1.2 will for the most part be used.

2.2.1 Conservation of mass

By interpreting χ as mass density ρ, and denoting the volume flux by $\vec{u}$, the mass flux becomes $\rho\vec{u}$ and Equation (2.6) represents mass conservation,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = q. \tag{2.12}$$

The concept of mass conservation is perhaps the most fundamental in continuum mechanics. With this as a foundation, governing equations for a large range of applications are formed, together with additional assumptions and constraints.

By assuming incompressibility, that is, that the mass density ρ is constant, which is often a reasonable assumption for water and many other liquids, mass conservation can be formulated as

$$\nabla \cdot \vec{u} = 0. \tag{2.13}$$

This is commonly referred to as the continuity equation. Since mass conservation forms the basis for governing equations in many continuum mechanics problems, a desirable property of any solution strategy for these problems is that mass conservation is honored.

2.2.2 Conservation of momentum

If χ represents momentum, it can be replaced by $\rho\vec{u}$ and equation (2.6) represents momentum conservation,

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u}\vec{u}) = q \,. \tag{2.14}$$

The product of the flux vectors $\vec{u}\vec{u}$ is a dyad. This form of momentum conservation, where the domain Ω is assumed to be fixed in space, provides the Eulerian form of the conservation principle.

In many applications it may be more convenient to let Ω follow the motion of the material, or fluid. Then Ω is denoted a material volume and an integral form of Newton's 2nd law will provide the Lagrangian form of the momentum conservation principle, that is, the rate of change of momentum is balanced by the forces acting on the volume. These forces can be divided into body forces, with gravity as a typical example, and surface forces, also denoted as stress. This can be expressed as

$$\rho \frac{Du_i}{Dt} = \rho g_i + \frac{\partial \tau_{ij}}{\partial x_j}, \tag{2.15}$$

where $\frac{D}{Dt} = \frac{\partial}{\partial t} + \frac{\partial}{\partial x_i}\frac{\partial x_i}{\partial t} = \frac{\partial}{\partial t} + \vec{u} \cdot \nabla$ is the total derivative, Einstein's summation convention has been applied, and the subscripts i and j denote spatial directions. On the right hand side of equation (2.15), the vector g_i represents body forces, while the tensor τ_{ij} represents stress. Equation (2.15) is also known as Cauchy's equation of motion [112]. Sometimes, the primary interest is in the equilibrium configuration of the medium, which is described by omitting the time derivative term in Equation (2.15). This may be expressed on weak form, similar to as in Section 2.1.3: Find the displacement $\vec{x}$ such that

$$(\nabla \vec{y}, \tau(\vec{x})) = (-\rho \vec{g}, \vec{y}) \;\; \forall \, \vec{y} \in \mathcal{H}_0^1(\Omega). \tag{2.16}$$

2.2.3 Conservation of energy

For completeness, we mention another important conservation law used in continuum mechanics. Conservation of energy for a material volume,

$$\rho \frac{D}{Dt}\left(e + \frac{1}{2}u_i^2\right) = \rho g_i u_i + \frac{\partial}{\partial x_j}\left(\tau_{ij} u_i\right) - \frac{\partial q_i}{\partial x_i} \tag{2.17}$$

where e is the internal energy per unit mass and q_i is the ith element of the heat flux vector, describes the balance of mechanical and internal energy in the system. The mechanical energy is represented by the term $\rho \frac{D}{Dt}\left(\frac{1}{2}u_i^2\right)$. On the right hand side, the first and second terms represent the rate of work done by the body and surface forces, respectively, and the third term represents heat transfer. This law is derived from the 1st law of thermodynamics, which states that the total energy of an isolated system is constant, or that for a closed system, the change in internal energy equals the heat added to the system minus the work done by the system on the surroundings. When the internal energy is neglected, conservation of mechanical energy may be derived from momentum conservation [112].

3. Selected physical applications

In order to highlight different solution strategies for nonlinear problems in physical systems,it is useful to restrict the attention to a few selected applications. Specifically, we will consider nonlinear surface gravity waves, multiphase flow in porous media, and elastic deformation. These applications cover a range of systems with different interesting and challenging properties. For surface gravity waves, nonlinear equations with unusual properties turn out to be useful models, while for porous media heterogeneities, multiscale features, and data uncertainty pose great challenges. For nonlinear elasticity simulations, deformation of the physical domain is important to take into consideration.

The objective of this chapter is to outline how the governing equations for these problems arise from the mass and momentum conservation principles described in the previous chapter. For more detailed derivations of the equations, there is a rich litarature that may be consulted, see e.g. [12,43,112,167].

3.1 Surface gravity waves

Understanding the dynamics of water waves is important to coastal and river societies, where the energy contained in the waves can both be a threat to constructions on- and offshore and a potential resource. In this section, we will give a brief presentation of the dynamics of water waves. For a more comprehensive introduction, see e.g. [99,112,119,184] and the references therein.

Waves are motions due to a restoring force. If the restoring force is gravity, we have gravity waves. Figure 3.1 shows a sketch of surface gravity waves with an overview of some relevant quantities. Depending on the geometry and other assumptions on the physical system, different linear or nonlinear models may be applied. At the foundation of these models are the conservation laws described in the previous chapter.

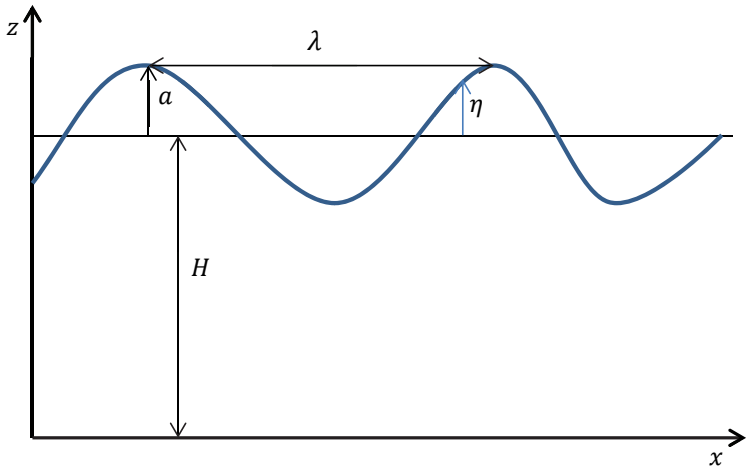

Figure 3.1: Conceptual sketch of surface gravity waves, including some relevant quantities: Displacement of free surface η, amplitude a, wave length λ and equilibrium depth H.

For certain types of surface waves in one dimension, a special nonlinear partial differential equation, the Korteweg-de Vries (KdV) equation [110,124], turns up. It may be formulated for the vertical displacement of the free surface, η, in terms of the long wave speed $c_0 = \sqrt{gH}$, where g is the gravitational acceleration, and the equilibrium water depth H:

$$\frac{\partial \eta}{\partial t} + c_0 \frac{\partial \eta}{\partial x} + \frac{3}{2}\frac{c_0}{H}\eta \frac{\partial \eta}{\partial x} + \frac{1}{6} c_0 H^2 \frac{\partial^3 \eta}{\partial x^3} = 0. \tag{3.1}$$

For the purpose of mathematical and numerical analysis, it is common to transform the equation to a form with unit coefficients. Using subscript notation for derivatives, the KdV equation then becomes:

$$\eta_t + \eta_x + \eta\eta_x + \eta_{xxx} = 0. \tag{3.2}$$

By introducing the flux $u(\eta) = \eta + \frac{1}{2}\eta^2 + \eta_{xx}$, this may be expressed as a conservation law for η,

$$\frac{\partial \eta}{\partial t} + \frac{\partial u}{\partial x} = 0, \tag{3.3}$$

which is the one-dimensional variant of Equation (2.6) with vanishing source term.

The KdV equation has proved to describe well e.g. solitary waves along a uniform canal [147] or undular bores that result from tidal waves entering certain tract-shaped river mouths [16,140]. Solitary waves, or solitons, are localized travelling waves of uniform shape and size, even when interacting with other solitons, except for a possible phase shift. The KdV equation has also been found to be a useful model for a variety of other physical applications, and plays a major role in soliton theory [53,58,59,156,188].

In terms of the conservation concepts presented in the previous chapter, the KdV equation may be traced back to conservation of mass and momentum, along with the assumptions of fairly shallow water, small amplitude $a \ll \lambda$, and a nonlinear restoring force. Fairly shallow water is typically characterized by $0.05 < \frac{H}{\lambda} < 0.1$, where λ is the wavelength, and gives rise to dispersive forces [112].

The Boussinesq approximation [20] eliminates the vertical coordinate from the basic equations, which is useful when the primary interest is in the motion of surface waves, which propagate horizontally. The KdV equation then falls out as a balance equation between a nonlinear term (third term in equation (3.2)) and a dispersive term (fourth term), in addition to pure advection (two first terms).

The KdV equation has a variety of interesting properties for a nonlinear partial differential equation: It has analytical solutions in the forms of solitons and cnoidal waves [58], it is completely integrable and it satisfies infinitely many conservation laws [124], to mention a few. The analysis of this equation is an ongoing research topic. In Paper A, two different solution strategies for the KdV equation are compared and discussed.

3.2 Flow in porous media

Understanding the dynamics of flow in porous media is of importance to a large number of applications. Although the term 'porous media' can be applied to any solid material with an interconnected network of pores, we here restrict our attention to geological porous media, typically petroleum reservoirs and aquifers. Modelling flow in these porous media accurately is a complex issue, both due to many physical processes going on simultaneously and over a broad range of length and time scales, and to uncertainty in – or lack of – data on the porous formations. This leads to advanced mathematical and numerical models, requiring massive amounts of computational power for realistic simulations. Still, providing output of sufficient accuracy may be unaffordable in many cases.

The motivation for studying flow in geological formations is found in many different applications. Traditionally, oil and gas production has been the main driver for research in this field. This is still the case, but it has been increasingly accompanied by other fields such as geothermal energy and CO2 storage in the past couple of decades. Other relevant fields are groundwater flow and waste management.

In the case of oil production, detailed knowledge about reservoir fluid flow has become increasingly important, as production techniques have grown more advanced and more fields have entered a mature stage. For new oil fields, the pressure in the reservoir is usually high enough to drive production alone (primary production). As the natural pressure support decreases, it is common to inject water, gas, high pressure air [40] or other substances in order to elevate the pressure or enhance fluid flow properties in order to increase the production further (secondary and tertiary production). Numerical models of the reservoir flow may act as a decision support tool for choosing production strategies and placing wells.

As the awareness of the connection between anthropogenic CO_2 emissions and climate change has grown, the need for renewable energy resources has become more and more evident. Geothermal energy has received increasing attention as there are vast amounts of energy stored as heat in the earth crust [74]. In this field, thermal

effects and flow through fractured porous media are important aspects that need to be understood. Another effort that is being held up as a way of reducing CO_2 emissions to the atmosphere is the capture and storage of CO_2 in geological formations [96]. These formations may be saline aquifers, unminable coal seams, old oil reservoirs, or producing oil reservoirs, as part of a secondary production strategy. Mathematical and numerical modelling is necessary in order to predict the movement of the injected plume of CO_2, in order to estimate formation capacity and assessing leakage risks [46,134].

Groundwater contained in porous aquifers constitutes around 30 % of the freshwater resources in the world [157]. Understanding of how the water flows through these formations is important for efficient water management, and to avoid or monitor contamination of the water.

In order to gain a deep understanding of flow and transport in geological porous media, advanced numerical simulators play a crucial role. Due to the large scales involved, laboratory tests are of limited use. The simulator may then act as a virtual laboratory, where test cases spanning hundreds of kilometers and thousands or even millions of years can be run. However, the validity of such tests relies on the quality not only of the data, but also on the mathematical and numerical models and the solvers used. Unfortunately, the equations describing flow in realistic porous media are generally extremely ill-conditioned, and no universal solution technique that consistently gives a reliable answer within a reasonable time-frame exists. The characteristic features of the governing equations may be highly different in different cases, depending on the dominating physical processes in each case. This serves as a driving force for further research on modeling and simulation of flow in porous media, where effort is divided between improvement on physical models, discretization, solvers and other aspects. Two other aspects that complicates the situation is that the rock properties are generally highly heterogeneous and highly uncertain, leaving little hope of obtaining an accurate and reliable solution of the problem.

In the remainder of this section, we will give a brief presentation of key concepts and equations related to flow in porous media. More detailed presentations may be found in e.g. [1,12,15,43]

3.2.1 Rock physics

The porosity is a dimensionless quantity that represents the fraction of void volume to total volume,

$$\phi = \frac{V}{V_{tot}}, \tag{3.4}$$

in a representative elementary volume (REV) of the rock. An REV is assumed to be at a scale where moderate changes to the volume do not change the parameters, significantly larger than pore scale and significantly smaller than the reservoir scale. On this scale, the porous medium may be treated as a continuum. An REV scale may not always exist, but we will assume it to be the case here. A modified definition of porosity, which is of more practical use in flow applications, follows from letting V only represent the connected pores. If the porous medium is completely filled with fluid, V also denotes the total fluid volume.

Another essential parameter in porous-medium flow is the permeability, which quantifies how easily fluid flows through the medium. The permeability is a symmetric positive definite tensor [4], which may be written in matrix form as

$$K = \begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{xy} & k_{yy} & k_{yz} \\ k_{xz} & k_{yz} & k_{zz} \end{bmatrix}. \tag{3.5}$$

The form of the tensor may be simplified by letting the grid align with the principal directions of the permeability, which leads to a diagonal tensor. Further simplification is possible by assuming equal permeability in all directions, in which case the permeability is reduced to a scalar value. However, in reality, the permeability in the vertical direction often differs significantly from the horizontal permeability. The SI unit of permeability is m^2, but often units of Darcy (or milliDarcy, mD), where 1

Darcy = $9.869233 \cdot 10^{-13}$ m^2, are used. In realistic geological porous media, the permeability may vary over several orders of magnitude over small distances. This is one of the major challenges in reservoir simulation, since these small scale variations may have a substantial impact on large scale flow patterns.

It is common to assume the rock properties to be constant with respect to time, which often is a good approximation. In reality, however, the rock may compress or decompress with changes in the overburden pressure, e.g. due to production or injection. Also, in fracking and enhanced geothermal systems, part of the process is to create fractures in the rock in order to facilitate flow [88,122].

3.2.2 Fluid properties

The fluids most commonly encountered in porous rock formations may be classified as water, oil and gas. The phases may each consist of a number of different components. In this work, we will only consider the phases and neglect the compositional aspects.

The density ρ of a fluid is defined as fluid mass per unit volume, that is,

$$\rho_i = \frac{m_i}{V_i} \tag{3.6}$$

for phase i. In general, the density of the fluid depends on other state variables such as pressure p and temperature. This dependency may be described through an equation of state, see e.g. [139,161]. Neglecting thermal effects, the compressibility may be defined as

$$c = \frac{1}{\rho}\frac{\partial \rho}{\partial p}. \tag{3.7}$$

For ideal fluids, the compressibility is constant, and by assuming the fluids to be incompressible it becomes zero. The latter assumption significantly simplifies the governing equations. For many liquids, including water, and to some extent oils, this

may be a good approximation. Gases, on the other hand, are highly compressible and need to be treated as such.

The viscosity μ of a fluid describes its resistance to flow due to internal friction on the molecular scale. For Newtonian fluids this does not depend on the shear rate or velocity of the fluid, and in isotropic cases it may be denoted by a scalar value μ.

3.2.3 Single-phase incompressible flow

Single-phase flow in porous media is on the continuum scale modelled using Darcy's law [52], which gives the volumetric fluid flow rate $\vec{u}$ as a function of the permeability and the pressure,

$$\vec{u} = -\frac{1}{\mu}K(\nabla p + \rho g \nabla z), \tag{3.8}$$

where z is the vertical coordinate. The second term represents the hydrostatic pressure gradient. Combining this with the incompressibility assumption and the mass conservation equation given in Section 2.2.1, this gives

$$-\nabla \cdot \frac{1}{\mu}K(\nabla p + \rho g \nabla z) = q, \tag{3.9}$$

or simply

$$-\nabla \cdot \vec{u} = q. \tag{3.10}$$

Equation (3.9) is an elliptic partial differential equation for p. The time derivative in the conservation law vanishes due to the assumption of incompressibility.

3.2.4 Multiphase flow

For multiphase flow, an extension to Darcy's law that takes phase mass distribution into account is necessary. Two new concepts need to be introduced in order to accomplish this; capillary pressure and relative permeability. These are typically modelled as a function of phase saturation, $s_i = V_i/V$, and often also of flow history, or hysteresis.

The relative permeability κ_i quantifies how the different phases flow relatively to each other. Common relative permeability models include the Brooks-Corey [27] and van Genuchten [73] models. The relative permeabilities satisfy $\sum_i \kappa_i \leq 1$. A related quantity to the relative permeability is the phase mobility,

$$\lambda_i = \frac{\kappa_i}{\mu_i}. \tag{3.11}$$

With the total mobility defined as $\lambda_T = \sum_i \lambda_i$, the fractional flow function may be defined for each phase as

$$f_i = \frac{\lambda_i}{\lambda_T}. \tag{3.12}$$

The capillary pressure in a two-phase system is defined as the difference between the pressures of the phases,

$$p_{cap} = p_w - p_{nw}, \tag{3.13}$$

where subscripts w and nw denote wetting and non-wetting phases, respectively. The Brooks-Corey and van Genuchten frameworks provide commonly used models also here.

The multiphase version of Darcy's law can then be formulated for each phase as

$$\vec{u}_i = -\lambda_i K\left(\nabla p_i + \rho_i g \nabla z + \nabla p_{cap}\right), \tag{3.14}$$

Simpler versions may be obtained by neglecting gravity and/or capillary effects, which in some cases may be reasonable assumptions. A set of partial differential equations that describes an incompressible two-phase system may be obtained by formulating conservation laws for mass for each phase. The mass per unit volume of phase i is $\phi s_i \rho_i$. The densities are cancelled as in the single-phase equation, but a time derivative remains in the mass conservation equation for each phase:

$$\phi \frac{\partial s_i}{\partial t} + \nabla \cdot \vec{u}_i = q_i, \tag{3.15}$$

Together with constitutive relations for relative permeabilities and capillary pressure, the system of partial differential equations (3.15) may be solved for one phase saturation and one phase pressure, with the additional assumption that the phases fill the entire pore space,

$$\sum_i s_i = 1. \tag{3.16}$$

Often, it is more practical to reformulate the problem to different forms than the fully coupled formulation (3.15). One example is found by summing the equations to obtain

$$-\nabla \cdot \vec{u}_T = q_T, \tag{3.17}$$

where $\vec{u}_T = \sum_i \vec{u}_i$ and $q_T = \sum_i q_i$. The time derivative vanishes due to Equation (3.16), and the same equation form as in the single phase problem is obtained. The total velocity may be expressed in terms of a global pressure $\bar{p}$ [42],

$$\vec{u}_T = -\lambda_i K \left(\nabla \bar{p} + \sum_i \rho_i g \nabla z \right), \tag{3.18}$$

which eliminates the explicit dependence of the total velocity on the capillary pressure. An alternative system of equations is then formed from equation (3.17) and one of the equations (3.15). This more weakly coupled formulation, known as the fractional flow formulation [39,42], clearly displays the elliptic-hyperbolic nature of the problem, as Equation (3.15) is hyperbolic with respect to saturation and Equation (3.17) is elliptic with respect to pressure.

Different solution strategies for nonlinear two-phase flow problems in porous media are the topics of Papers B and C.

3.3 Elasticity

Many physical processes include deformation of some kind. The deformation of an object is due to some applied force, and is elastic if the object returns to its original shape after the force is released. Other major kinds of deformation include plastic deformation and fracturing, which as opposed to elastic deformation are irreversible.

Examples of elastic deformation include stretching of rubber bands, trees and grass swaying in the wind, and steel springs. Elasticity of materials is also important to consider in construction projects. Poroelastic models [17,179] are used in applications where the deformation of a porous material is of importance, including rock formations and human tissue.

This section will provide a very brief description of linear and nonlinear elasticity, as it would be beyond the scope of this study to go deeply into the details. The reader is referred to the material presented in e.g. [106,136,150,167,191] for a more in-depth presentation.

The most basic physical model of elastic deformation is the linear elasticity model, where the deformation is assumed to be a linear function of the applied force. Linear elasticity is based on an assumption of small deformations. The relation between applied force and displacement is then described by Hooke's law, which may be expressed in terms of the Cauchy stress tensor τ and strain tensor ϵ as

$$\tau = C\epsilon, \tag{3.19}$$

where C is the fourth order stiffness (or elasticity) tensor. In the isotropic case, C is scalar and known as Young's modulus. The strain tensor may be expressed in terms of the deformation $\vec{x}$ as

$$\epsilon(\vec{x}) = \frac{\nabla\vec{x} + \nabla\vec{x}^T}{2}, \tag{3.20}$$

that is, a symmetrized deformation gradient, which is composed of the derivatives of the displacement vector with respect to the reference configuration. It is often

convenient to use the equilibrium configuration as reference configuration, but any other configuration may in principle be used. For larger deformations, a nonlinear model is needed, as the original and deformed states of the material are significantly different. A material that allows expressing the stress tensor as a function of strain alone, is called a Cauhy-elastic material, and the stress-strain relation can be written on the form

$$\tau = G(\epsilon) \tag{3.21}$$

where G is a nonlinear tensor mapping. Hooke's law is a special case of this relation. For other materials, e.g. hyper- and hypoelastic materials, the linear model is insufficient even for small deformations [167,172]. We will not discuss these further here.

A set of governing equations for nonlinear elasticity problems may be obtained from Equations (3.20) and (3.21) above and a conservation law for momentum. In order to describe the displacement of each particle in the deforming medium, a Lagrangian description of the system is a natural choice. For the equilibrium configuration, and using the weak form (2.16), this becomes the problem of finding $\vec{x} \in \mathcal{H}_0^1(\Omega)$, such that

$$\big(\epsilon(\vec{y}), \tau(\vec{x})\big) = (-\rho\vec{g}, \vec{y}) \quad \forall\, \vec{y} \in \mathcal{H}_0^1(\Omega), \tag{3.22}$$

with $\tau(\vec{x})$ determined by Equation (3.21).

The finite strain theory provides a framework for arbitrarily large deformations. Different kinds of stress measures may be convenient in such cases, e.g. the Piola-Kirchhoff stress tensors which relate the stress in a deformed configuration of the medium to the reference configuration [167]. The first Piola-Kirchhoff stress tensor is defined as

$$\tau_{PK1} = \det F\, \tau \cdot F, \tag{3.23}$$

where $F = \nabla\vec{u}$ is the deformation gradient tensor. For a more comprehensive presentation of this subject, see e.g. [167,191].

Solution strategies for a nonlinear elasticity problem is presented and discussed in Paper D.

4. Discretization methods

In the previous chapter some mathematical models for different physical phenomena are outlined. These continuous models cannot be handled directly by computers, which only operate on discrete data. Therefore, the models need to be discretized, such that the properties involved are defined only on a finite number of points rather than on continuous regions. The subject of discretization is very wide, and there is a rich literature on different discretization methods, see e.g. [118,145,151,192].

The optimal choice of discretization depends largely on the problem at hand, as different methods have different advantages and disadvantages. For instance, elliptic and hyperbolic problems differ in the sense that elliptic problems are globally coupled, while hyperbolic problems have local couplings and finite propagation speeds. Also, the KdV equation has properties not found in the saturation equation (3.15) and vice versa, although both are hyperbolic. The elasticity problem in Section 3.3 follows a Lagrangian description, while the other problems discussed in this work have an Eulerian setup. These and other differences should be reflected in the discretization methods. The literature is richer on spatial discretization methods, although several different temporal discretization techniques are available. This reflects the fact that the differences in the continuous equations are largely found in the spatial terms. In this chapter, short presentations of four classes of spatial and one class of temporal discretization methods are given.

4.1 Spatial discretization

This section provides presentations of different discretization methods that are commonly used for the physical systems described in the previous chapter, and some discussion regarding why they are natural choices in the respective cases.

Some important properties of discretization methods are consistency, stability and convergence. A discretization is said to be consistent if the discretized equations are reduced to the continuous equations as the grid point distance $h \to 0$. If the

approximation error is bounded, the method is stable. The Lax-Richtmeyer equivalence theorem [116,118] states that a discretization that is consistent converges if and only if it is stable. These properties, along with conservation properties, are important to consider when choosing a discretization scheme.

4.1.1 Finite difference methods

The finite difference methods are among the simplest discretization methods available. Their simplicity in form has made them popular across many application fields. The methods are based on approximations of derivatives in the governing partial differential equations, based on the definition of the derivative. These methods are most commonly used on rectangular grids, but triangular and hexagonal grids may also be used. Formulating the methods on more general grid forms is an elaborate task, so the practical use of finite difference method is limited to regular grids. Hence, the methods are most efficient on applications that do not require complex grid geometries.

The approximation of a derivative at a certain grid point is determined by function values at a limited number of neighboring points, with the number of points used depending on the desired accuracy and the order of the derivative. The formulas are based on Taylor expansions,

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f''''(x) + \cdots, \tag{4.1}$$

and

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f''''(x) - \cdots, \tag{4.2}$$

of the function f around a certain point, here x, with a small scalar value h, which may be positive or negative. For instance, the derivative of a function, $f'(x)$, may be approximated by rearranging Equation (4.1),

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h), \tag{4.3}$$

or Equation (4.2),

$$f'(x) = \frac{f(x) - f(x-h)}{h} + O(h), \tag{4.4}$$

providing two one-sided schemes. Here, h represents the distance between neighboring grid points. The $O(h)$ term indicates that the convergence rate of the approximation error as $h \to 0$ is of first order. By combining formula (4.1) with the corresponding formula for $-h$ to obtain

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2), \tag{4.5}$$

a central scheme of second order occurs. Higher order derivatives may be calculated similarly. Involving more points on each side may generate higher order schemes [72]. However, the more points that have to be evaluated, the more costly the scheme. Finite difference methods are easily applied to multi-dimensional problems by applying the schemes on the different partial derivatives involved in the equations.

These schemes result in sparse banded matrices representing the derivative term for the whole discrete domain. The lack of flexibility in grid forms is a drawback for these methods when the geometry of the problem is irregular. Also, convergence rates may be slow compared to other methods.

The one-sided difference schemes above are especially useful for hyperbolic problems where the solution propagates in one direction and the solution at a grid point is only based on information from one side. For linear hyperbolic equations this is straightforward to implement. For more complex problems where the flow direction may change, such as in two-phase flow in porous media, it is necessary to

automatically detect the flow direction and use information from the upstream cell. This is known as upstream differencing [26,152], and is applied to the hyperbolic saturation equation in Papers B and C.

4.1.2 Spectral methods

Spectral methods [37,141,170] are constructed from a set of global basis functions that are weighted using scalar coefficients. The discrete problem then consists of finding weights that make the sum of basis functions approximate the true solution within a given tolerance level. The global nature of these functions leads to dense coefficient matrices. On the other hand, these are typically smaller than the matrices corresponding to other methods such as the finite difference method. This is because spectral methods require fewer grid points to obtain a certain accuracy due to the excellent convergence properties, often denoted spectral convergence.

We will restrict the discussion of spectral methods to bounded, one-dimensional domains. Two important classes of spectral methods are the Fourier methods, which use trigonometric interpolation functions on uniform grids, and Chebyshev methods, which use the Chebyshev polynomials as interpolating functions on grids based on the so-called Chebyshev points. An alternative polynomial approach is based on the Legendre polynomials.

In either case, the derivatives in the governing equations are evaluated in terms of derivatives of the basis functions. Since the basis functions have global support, the corresponding coefficient matrices become dense. This unattractive feature is largely outweighed by the spectral convergence rate, which is exponential with respect to grid resolution, assuming the solution is sufficiently smooth. This is in contrast to e.g. finite difference methods that have polynomial order of convergence. A drawback for many applications is the rigidness of the grid point locations.

The Fourier method is well-suited for periodic problems, given the form of the interpolating functions, although it is also possible to use it for non-periodic problems e.g. if the interesting part of the solution is kept away from the boundaries. A

phenomenon that occurs for discontinuous solutions is the Gibbs phenomenon, which is an overshooting oscillation phenomenon near the discontinuities.

For non-periodic problems, the Chebyshev method is a popular choice. The Chebyshev points are defined as the extreme points of the Chebyshev polynomials, defined recursively as

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad n \geq 1 \tag{4.6}$$

with $T_0(x) = 1$ and $T_1(x) = x$. An equivalent definition of the Chebyshev points is

$$x_j = \cos\left(\frac{j\pi}{N}\right), \qquad j = 0,1, \dots, N, \tag{4.7}$$

where N is the number of grid points. This can be visualized as the projection of equidistant points on the unit circle to the x-axis. Hence, the points are densely distributed near the boundaries of the interval $x \in [-1,1]$ and more sparsely in the central parts. This has the effect of minimizing the Runge phenomenon, that is, large non-physical oscillations near the boundaries of the domain that occur when interpolating smooth functions with polynomials on equispaced points [51]. It may be shown that an optimal density of grid points satisfies

$$\rho_{\text{grid}}(x) = \frac{1}{\pi\sqrt{1-x^2}}, \qquad x \in [-1,1] \tag{4.8}$$

This is the case with the Chebyshev points [170], as may be verified from the definition of the points.

The Chebyshev method is related to the Fourier method in the sense that the interpolating functions are transformed trigonometric functions, cf. Equation (4.7). Consequently, Fourier analysis is relevant for both methods. This includes the use of the Discrete Fourier Transform (DFT), which transforms functions from physical space to frequency space in order to obtain the coefficients in the Fourier series. The Fast Fourier transform (FFT) [48], is a class of efficient algorithms for calculating the DFT.

While Fourier methods are frequently used for the KdV equation, this is not the case for Chebyshev methods. However, for problems with non-homogeneous Dirichlet boundary conditions, Chebyshev methods may appear as a more attractive alternative. In Paper A, the performances of a Chebyshev spectral method and a finite difference method are compared.

4.1.3 Control volume methods

Control volume (CV) methods [2,5,63,64] are based on the integral form of the governing equations. This class of methods is designed to retain the conservation properties of the continuous equation in the discretization. This is done by dividing the domain into smaller cells, or control volumes, on which the conservation principle is applied. These cells may have arbitrary polyhedral shapes. At the heart of the method is the calculation of fluxes on each face of the volume.

The CV methods are especially suitable to elliptic or near-elliptic problems such as the single phase flow equation (3.9) or the pressure equation in the two-phase flow problem, which are expressions for mass conservation for flow in porous media. Consider a slightly simplified version of these equations,

$$-\nabla \cdot K\nabla p = q. \tag{4.9}$$

Darcy's law accordingly gives the flux as

$$\vec{u} = K\nabla p. \tag{4.10}$$

The flux $\vec{u}$ is proportional to the pressure drop ∇p. Let the pressure values be represented in the cell centers, and assume the permeability tensor K to be constant within each cell. The simplest form of CV is obtained by letting the fluxes across each edge based on the pressure differences between the cells corresponding to that edge, along with a harmonic mean of the permeabilities. This gives the following expression for the flux across the face separating cells i and $i+1$ in the x-direction:

$$\vec{u}_{i,i+1} = -\gamma_{i,i+1} \frac{p_{i+1} - p_i}{\frac{1}{2}\left(\frac{\Delta x_i}{k_{1,i}} + \frac{\Delta x_{i+1}}{k_{1,i+1}}\right)} \tag{4.11}$$

Here, $\gamma_{i,i+1}$ is the area of the face between the cells. This is commonly referred to as Two-Phase Flux Approximation (TPFA). This method is limited to K-orthogonal grids, that is, grids in which straight lines between neighboring cell centers align with the principal directions of K. This yields simple expressions, which again has made this method very popular and widely used in reservoir simulators. However, this criterion also limits its usability on general grids, such as grids aligning with features in the permeability field.

In order to work on general grids, the natural extension of TPFA is the Multi-Point Flux Approximations (MPFA) methods. As the name suggests, each flux is calculated based on multiple points. There are several different MPFA methods, including the L-method, which uses three points, and the O-method, which uses four points. This makes the methods more robust, and applicable on general grids. The combination of flexibility with gridding and mass conservative schemes has made these methods popular for simulations of flow in porous media, where these properties are critical. However, these methods have some issues with monotonicity. While the continuous equation (4.13) satisfies a maximum principle, this is challenging to obtain for the discrete equation with an MPFA method [102,131,132]. The formulations of the methods are also somewhat more complex and computationally more demanding than for TPFA. There is no comprehensive theory for the convergence of the CV methods, although convergence is proved for some cases [4].

The TPFA method is applied for the elliptic pressure equation in Papers B and C.

4.1.4 Finite element methods

Another important class of spatial discretization methods is the Finite Element Methods (FEM) [14,164,192]. These methods are based on dividing the domain into a non-overlapping set of smaller elements and representing the solution using basis functions with local support. This is similar to the spectral methods described above,

except that the basis functions are local here, in contrast to the global basis functions of the spectral methods. Each node, or intersection point between different element edges, has one basis function associated with it, and the weighting of the functions determines the solution. By specifying different types of elements and basis functions, different methods may be obtained.

FEM is based on the weak formulation of the governing equations shown in section 2.1.3. An equivalent problem to Equation (2.9) is the minimization problem

$$\min_{u \in \mathcal{H}_0^1(\Omega)} L(u), \tag{4.12}$$

where

$$L(u) = \frac{1}{2} b(u,u) - (q,u), \tag{4.13}$$

with $b(\,,)$ and the inner product $(\,,)$ defined as in Section 2.1.3. In order to obtain a discrete version of the problem, the Ritz-Galerkin method may be used. This approach makes use of finite-dimensional test functions $v_h \in \mathcal{V}_h$, where $\mathcal{V}_h$ is the space of nodal basis functions for $\mathbb{P}_k(\Omega_h) \subset \mathcal{H}_0^1(\Omega)$. Here, $\mathbb{P}_k(\Omega_h)$ is the set of polynomials of degree k or less on Ω_h, the discretized version of Ω. That is, find the $u_h \in \mathcal{V}_h$ that satisfies

$$\frac{1}{2} b(v_h, u_h) = (q, v_h), \tag{4.14}$$

for all $v_h \in \mathcal{V}_h$. It may be shown that $u - u_h \perp \mathcal{V}_h$. Here, the subspaces for test functions, v_h, and trial functions, u_h, has been chosen to be the same, $\mathcal{V}_h$, but they may also be chosen to be different. With the choice above, $\mathcal{V}_h$ is the space of piecewise polynomial functions up to degree k. A common choice, and the simplest option, is to set $k = 1$. This yields piecewise linear basis functions, also known as hat functions. Quadratic and higher degree polynomials may also be used in a straightforward manner, but more points are required to define the basis functions then.

FEM are extremely popular for a wide range of disciplines, including elasticity. Part of the popularity is due to the flexibility in grids, which is important in many applications. In elasticity problems this is particularly attractive as the physical domain deforms. A large part of the popularity also stems from the relaxed smoothness criteria due to the weak formulation and the ability to represent arbitrary functions in a function space using local basis functions. We have employed a FEM discretization for the elasticity problem in Paper D.

In the case of porous media problems, the lack of mass conservation limits the applicability of the method. Also, the permeability tensor is arithmetically averaged in FEM, which is a problem if the average is to be taken across a discontinuity, which is the case with element-wise constant permeability. Harmonic averaging, such as in CV methods, would yield a better representation of the actual effective permeability.

The convergence rate depends on the grid properties and the basis functions. A discussion of the convergence using the Ritz-Galerkin approach with linear basis functions can be found in [4].

4.2 Temporal discretization

For equations with time dependence, the temporal terms need to be discretized as well. Usually, the temporal dimension is discretized separately from the spatial dimensions. A useful model problem for discussing temporal discretization is the general form

$$\frac{\partial u}{\partial t} - f(\vec{x}, t) = 0. \tag{4.15}$$

We will only consider finite difference representations here, as this is by far the most common choice, and other discretization methods are of less practical use for time stepping.

The natural approach to a time-dependent problem is to start from an initial time t_0 and calculate the system state at incremental steps $t_1, t_2, \dots, t_{max}$. There are two main

directions from here, namely implicit and explicit time-stepping methods. For explicit methods, the state at a point x_i at time t_{n+1} depends only on values from time steps up to t_n, that is, known values. For implicit methods, the state at x_i also depends on values from the current time step, t_{i+1}, thus requiring the solution of a system of equations on each time step. The remainder of this section discusses general properties of these classes of time stepping methods, as well as some specific examples of methods.

4.2.1 Explicit methods

With explicit time-stepping methods, the state at a point in space at a time step can be expressed as a function of known quantities, calculated at previous time steps. This is favorable from a computational perspective. However, there may be strict criteria for stability involved, and this may put severe limitations on the time step length Δt, possibly outweighing the low cost per step. The Courant–Friedrichs–Lewy (CFL) condition [49] relates Δt with the spatial grid point distance h and the velocity at which wave components of the solution travel. The Courant number is defined in the one-dimensional case as

$$C = |u_{max}| \frac{\Delta t}{h}. \tag{4.16}$$

Here, $|u_{max}|$ is the maximum magnitude of the velocity over the entire grid. The CFL condition may be stated as $C \leq C_{max}$, where C_{max} depends on the time-stepping method and the problem at hand. Typically, $C_{max} \leq 1$. This condition ensures that the physical domain of dependence is contained in the numerical domain of dependence. If the condition is not met, the numerical solution on the new time step suffers from a lack of necessary information, and may become unstable. Equation (4.16) is formulated for a one-dimensional problem, similar conditions may also be defined for multi-dimensional cases.

The most basic explicit time stepping method is known as the forward Euler method. This method approximates $\frac{\partial}{\partial t}$ at step $i+1$ by a simple difference formula using values from steps i and $i+1$,

$$\frac{\partial u}{\partial t} = \frac{u_{i+1} - u_i}{\Delta t} + O(\Delta t), \tag{4.17}$$

with the subscript denoting the time step, and evaluates all the spatial terms on step i. This gives the formula for u_{i+1} as

$$u_{i+1} = u_i + \Delta t f(x_i, t_i) + O(\Delta t^2), \tag{4.18}$$

The forward Euler method is a first order method, since the global error of a time-stepping method, defined as the difference between the true solution and the numerical solution, is one order smaller than the local truncation error. This is due to the fact that the number of time steps taken in order to reach a certain point increases with decreasing time step size.

Higher order methods, such as Adams-Bashforth methods, may be constructed by incorporating information from multiple time steps. By also including time step $i-1$, a method on the form

$$u_{i+1} = u_i + \Delta t \left(\frac{3}{2} f(x_i, t_i) - \frac{1}{2} f(x_{i-1}, t_{i-1}) \right) + O(\Delta t^3) \tag{4.19}$$

may be constructed. This is a second order method. Similar formulas may be constructed using information from more time steps, with the order of convergence increasing with one per time step included [82].

Several other strategies are available. The Leapfrog method evaluates the spatial derivatives on an intermediate step between the time steps involved in the temporal difference. The class of Runge-Kutta methods offer higher order methods, although at the cost of more complicated formulas.

4.2.2 Implicit methods

The backward Euler method is the implicit counterpart of forward Euler, with $f(x,t)$ evaluated at the current time step, $i+1$,

$$u_{i+1} = u_i + \Delta t f(x_{i+1}, t_{i+1}) + O(\Delta t^2). \tag{4.20}$$

As u_{i+1} here cannot be stated as a function of known quantities, a system of equations has to be solved on each time step. This may be very computationally expensive, especially for large grids. On the other hand, the stability properties are usually far superior to explicit methods, allowing for larger time steps. There may still be other factors, such iterative solvers failing to converge, that contribute to lowering the time step.

It is also possible to construct methods that combine the two approaches just outlined. An archetypical method is the trapezoidal or Crank-Nicolson scheme [50], which may be seen as a combination of the forward and backward Euler methods,

$$u_{i+1} = u_i + \Delta t \left(\frac{1}{2} f(x_{i+1}, t_{i+1}) + \frac{1}{2} f(x_i, t_i) \right) + O(\Delta t^3). \tag{4.21}$$

Second order convergence and excellent stability properties, including unconditional stability for e.g. the diffusion equation, makes this implicit method a popular choice in many applications [145].

5. Solution strategies

In the preceding chapters, some mathematical models of different physical systems and discretization methods have been described. This section will focus on forming efficient solution strategies by combining these with suitable iterative solvers for the linear and nonlinear systems of equations that arise. Trade-offs between different desirable properties are discussed.

While the governing equations in general are nonlinear, the solution techniques for these equations will result in systems of linear equations. We start by presenting some strategies for solving nonlinear systems, before moving on to linear solution strategies. At the end of this chapter, some strategies for solving time-dependent problems, linking spatial and temporal discretizations and strategies for nonlinear and linear systems, are discussed.

5.1 Solving nonlinear systems

The general nonlinear problem may be formulated as

$$F(u) = 0, \qquad u \in \Omega, \tag{5.1}$$

along with a set of boundary conditions on $\partial\Omega$. It is readily seen that the general linear problem is the special case where $F(u) = b - Au$. Finding solution strategies that work well for a general nonlinear problem is a challenging task, since all known strategies have some weak points. The best strategy is usually found by considering the specific features of the problem at hand and finding a method that addresses these features. This involves both taking advantage of features that may simplify the solution process and being especially careful with challenging features. For instance, in the special case of the KdV equation, exceptional features such as complete integrability and the existence of analytical solutions may lead to solution strategies that are unavailable to most other problems. As the KdV equation in this way forms an exception to the rule, most of this section will be devoted to the more general

nonlinear problems, but with special attention to the problem structures found in the physical systems described in Chapter 2.

For most nonlinear problems, the backbone of the solution strategy is linearization, usually by Newton iterations [57,103,137]. From this point, a linear solution strategy, discussed in the next section, may be applied. Different features of the nonlinear problem may guide the strategy, both on the nonlinear and the linear sides of the linearization process.

5.1.1 Newton's method

Newton's method is an iterative root-finding algorithm for general functions in arbitrary dimensions. This makes it well-suited for solving nonlinear problems, since Equation (5.1) is really a problem of finding the roots of the nonlinear function $F(u)$.

The mechanics of the algorithm may be explained in one dimension. Starting from an initial guess $u^{(0)}$, Newton's method calculates the derivative $F'(u^{(0)})$. The linear function intersecting $F\left(u^{(0)}\right)$ with slope $F'(u^{(0)})$ determines the next iterate, $u^{(1)}$ to be the point where the linear function is zero. Then $F'(u^{(1)})$ is calculated and the process is repeated until a root is found with sufficient precision. This gives the following formula for $u^{(k+1)}$:

$$u^{(k+1)} = u^{(k)} - \frac{F\left(u^{(k)}\right)}{F'(u^{(k)})}. \tag{5.2}$$

However, there is no guarantee that a root will be found at all, and in the case of multiple roots, at most one root will be found for each starting point $u^{(0)}$. In practice, uniqueness of the solution may often be assumed, which eliminates the latter concern.

In multiple dimensions, the equivalent of $F'(u)$ is the Jacobian $J(u)$, a matrix consisting of all the partial derivatives of all of the components of F with respect to all of the components of u. The iteration then takes the form

$$u^{(k+1)} = u^{(k)} - J^{-1}(u^{(k)})F(u^{(k)}) \tag{5.3}$$

This corresponds to solving the linear system

$$J\left(u^{(k)}\right)\Delta u^{(k+1)} = -F\left(u^{(k)}\right), \tag{5.4}$$

where $\Delta u^{(k+1)} = u^{(k+1)} - u^{(k)}$, at each iteration step. The analysis of multi-dimensional Newton iterations is not straightforward in the general case. It has however been proved that Newton's method converges quadratically under certain assumptions, that is,

$$\lim_{k\to\infty} \epsilon^{(k+1)} = c(\epsilon^{(k)})^2 \tag{5.5}$$

for the error $\epsilon^{(k)} = |u^* - u^{(k)}|$ and some constant c. One of the assumptions that needs to be met is that the initial guess must be in the convergence basin of that root. This is generally difficult to predict a priori. In order to improve this situation, globalization techniques such as linesearch or trust-region methods may be employed in order to expand the convergence basin [55,128].

For time-dependent problems, a nonlinear problem of the form (5.1) is to be solved on each time step. A common approach then is to reduce the initial time step length if the solution does not converge in a pre-defined number of iterations. After successful time steps, the time step length may again be increased, based on a suitable set of criteria.

In practice, the iteration process is stopped before the exact solution is found. This is partly due to the limitations of floating point arithmetic, and partly due to the fact that for many large problems, the cost of solving the linear systems on each Newton step is dominating the computational cost. Another aspect is that the exact properties of the physical system may be highly uncertain, and the models may also have been simplified to such a degree that going beyond a certain precision level in the numerical solvers may not improve the precision with respect to the physical problem, which ultimately is the most interesting one. This is indeed the case e.g. for

flows in geological porous media. Hence, convergence is declared when the error, based on a suitable measure, satisfies a certain tolerance τ,

$$\epsilon^{(k)} \leq \tau. \tag{5.6}$$

This is known as Inexact Newton iteration [54]. As the exact solution generally is unknown, the error may be represented e.g. by the residual, that is, $F(u)$. Alternatively the difference between two successive iterates may be used.

It should be noted that although J may be very large when resulting from a fine discretization of a problem of the type discussed in the previous chapters, it is usually sparse, with just a fraction of the elements nonzero. Still, evaluating the Jacobian explicitly may be difficult and multiplying it with vectors may be costly. In order to save computational time and memory, several techniques that eliminate the need for an explicit representation of J have been developed. These are known as Jacobian-free methods [109] and are motivated by the fact that for most linear solvers, J itself is not needed for solving the system, just the vector y resulting from multiplying it with another vector v,

$$y = Jv. \tag{5.7}$$

This is indeed the case for the Krylov methods presented in the next section, where v typically represents basis vectors for subspaces where a solution is sought.

In addition to the standard Newton's method, many other variants and similar methods exist, e.g. continuation Newton methods [6,187], Broyden's method and the secant method [103].

5.2 Solving linear systems

The general real linear system of n unknowns and n equations may be expressed as

$$Ax = b, \tag{5.8}$$

where A is an $n \times n$ matrix consisting of the coefficients a_{ij}, $x \in \mathbb{R}^n$ is the vector of unknowns and $b \in \mathbb{R}^n$ is the right hand side vector. Systems like this show up frequently in numerical models of physical systems, e.g. at each step in a Newton iteration, cf. Equation (5.4) in the previous section. The solution of Equation (5.8) is

$$x = A^{-1}b, \tag{5.9}$$

where A^{-1} is the inverse of A, defined by $A^{-1}A = I$. Calculating A^{-1} directly has a computational cost of $O(n^3)$ operations, meaning that for large systems, this is not a realistic option. Therefore, other strategies for solving linear systems are needed.

Solution methods for linear systems of equations can be categorized as direct or iterative. Direct methods solve the systems exactly using a finite number of operations while iterative methods approximate the solution by successively performing simpler operations based on certain rules. The latter may or may not converge to the true solution. There is a rich literature on solution methods for linear systems, see e.g. [75,84,103,117,145,171].

5.2.1 Direct methods

A direct method for solving linear systems of equations is a solution strategy that yields the exact solution in a finite number of steps, assuming exact arithmetic. For more than a handful of unknowns, it is crucial to automate the solution process of the system (5.8). The most commonly known direct approach is the Gaussian elimination, which consists of transforming the system to a triangular form by performing elementary row operations such as adding a row to another, multiplying a row by a scalar, and swapping positions of rows, and then finding the solution by back-substitution. When expressed on matrix form, this is known as the LU method or LU factorization, as it may be viewed as expressing A as the product of a lower-triangular matrix L and an upper-triangular matrix U,

$$LUx = b. \tag{5.10}$$

The system is then solved in two steps by first setting $y = Ux$ and solving

$$Ly = b \tag{5.11}$$

for y by forward substitution and then solving

$$Ux = y \tag{5.12}$$

for x by back substitution. For small matrices the LU method and variants thereof are widely used. Note that the borderline between small and large matrices is rather diffuse and has been moving with the developments in computing resources.

5.2.2 Iterative methods

The LU method needs $O(n^3)$ operations, and is thus generally computationally expensive as n grows. The situation is similar for other direct methods, so a different approach is needed for large systems of equations. Iterative methods compute an approximate solution from an initial guess and a set of rules for advancing to the next iteration step. Among the more basic iterative methods are the Jacobi and Gauss-Seidel methods, which belong to the class of stationary iterative methods. In order to describe some more advanced iterative methods, it is useful to start out from another simple stationary method, the Richardson iteration, which computes the solution at step $k + 1$ using the formula

$$x^{(k+1)} = b + (I - A)x^{(k)}. \tag{5.13}$$

This may be written in terms of the residual $r^{(k)} = b - Ax^{(k)}$,

$$r^{(k+1)} = (I - A)r^{(k)} \tag{5.14}$$

The initial guess will here be assumed to be $x^{(0)} = 0$. This does not imply any loss of generality, as the system of equations otherwise easily can be translated into a system with zero initial guess. Then, by the recursion formula,

$$\begin{aligned} r^{(k+1)} &= (I - A)^{(k+1)} r^{(0)} \\ &= P_{k+1}(A) r^{(0)} \\ &= P_{k+1}(A) b \end{aligned} \tag{5.15}$$

where $P_{k+1}(A)$ denotes a polynomial of order $k+1$. In other words, the residual anywhere in the iteration can be expressed as a polynomial with degree corresponding to the iteration counter. In terms of x this relation reads

$$x^{(k+1)} = \sum_{i=0}^{k} P_i\,(A) b. \tag{5.16}$$

In light of this observation, it is natural to seek solutions of the type

$$x^{(k)} \in \mathcal{K}^k(A; b) = \text{span}\{b, Ab, A^2 b, \dots, A^{k-1} b\}. \tag{5.17}$$

The space $\mathcal{K}^k(A; b)$ is called the Krylov subspace of order k with respect to A and b. When the meaning is clear from the context, the shorthand $\mathcal{K}^k$ is often used. Since $\mathcal{K}^n$ spans $\mathbb{R}^n$, it must contain the exact solution.

There are different strategies that can be employed in order to find the solution using the Krylov subspaces. Here, we will give a brief description of some of the most widely used Krylov methods. For a more detailed presentation, see e.g. [80,103,148,176]. The vectors $\{b, Ab, \dots, A^k b\}$ do not comprise a suitable basis for $\mathcal{K}^k$, as for large k the last vectors tend to point more and more in the same direction, making them undistinguishable in finite precision at some point. An orthonormal set of basis vectors may be composed through the Arnoldi process [11], which employs either the Gram-Schmidt process or Householder transformations [87] for orthogonalization. Let the columns of the matrix V_k be the resulting orthonormal basis vectors. The kth step of the Arnoldi process may be expressed in matrix form as

$$AV_{k-1} = V_k H_{k,k-1}, \tag{5.18}$$

where $H_{k,k-1}$ is a $k \times k-1$ upper Hessenberg matrix whose elements h_{ij} are computed in the orthogonalization process. An upper Hessenberg matrix is a matrix

with nonzero elements only at and above the first subdiagonal. Alternatively, one may write

$$V_k^T A V_k = H_{k,k} \tag{5.19}$$

where $H_{k,k}$ is the $k \times k$ matrix constructed by appending the coefficients computed at step k to $H_{k,k-1}$.

From this point, different approaches are possible, depending on the properties of the problem and practical constraints such as available computer memory. For symmetric positive definite problems, the method of choice is usually the Conjugate Gradients (CG) method [68,83,114]. For non-symmetric problems, there is no universally optimal method [125], and choosing the best method for a specific problem is not trivial. Numerous methods with different advantages and disadvantages exist, but very often the choice falls on some variant of either the Generalized Minimal RESidual (GMRES) method [149,177] or the Bi-Conjugate Gradients stabilized (BiCG-stab) method [175]. Unlike many other methods, these are applicable to general matrices and have proven to be efficient for large classes of systems [171,175]. A major difference between these two methods is that GMRES is based on the long-recurrence Arnoldi orthogonalization process [11], while BiCG-stab is based on the short recurrence Lanczos bi-orthogonalization process. The latter clearly has the advantage of low storage requirements, but has an irregular convergence rate. GMRES converges monotonically, but in its native form it requires storage of vectors corresponding to every iteration step throughout the iteration process.

GMRES is, as indicated by the name, a residual-minimizing method, i.e., on step k, it finds the vector in $\mathcal{K}^k$ that minimizes the norm of the residual, $\|r^{(k)}\|$. A consequence of this is that in at most n steps, the exact solution is found. In this sense it may be argued that GMRES is a direct method, but for all practical applications the iteration is truncated long before reaching this point, due both to limitations in computational power and in attainable precision in floating point arithmetic. The growing memory costs at each step are usually handled by restarting the iterations

every m steps, denoted the GMRES(m) algorithm [148]. Restarting comes with a risk of stagnation, however, and the choice of m, is often a matter of trial and error.

Since the CG method is the superior method for symmetric positive definite systems, it is natural to attempt to bring some of the qualities over to the more general case of nonsymmetric systems. The Bi-Conjugate Gradient method (BiCG) is a generalization of CG which allows for short Lanczos-based recurrences for nonsymmetric systems. BiCG-stab is a faster and more robust variant of BiCG [71,115]. The basis vectors are here bi-orthogonal, while in CG they are orthogonal. Despite the improvement in robustness from BiCG to BiCG-stab, the convergence is not monotonical and not even guaranteed. Further enhancements aiming to remedy these issues have been made, see e.g. [79,159]. Another class of methods is the Induced Dimension Reduction (IDR) methods, which are closely related to BiCG methods, although developed from a different perspective [158,162,183].

For any Krylov method it should be noted the convergence rate is sensitive to the condition of the system. As many relevant problems are ill-conditioned, the methods are rarely used without preconditioning, that is transforming the original problem to an equivalent one with better condition. This subject is discussed further in the next chapter.

5.3 Strategies for time-dependent problems

For time-dependent problems, there are numerous possible ways of combining equation formulations, discretizations, and solvers. For coupled problems, there is also the choice of how to handle the couplings. In this section, some strategies for solving the KdV equation and the coupled problem of two-phase flow in porous media will be discussed.

5.3.1 Time-stepping strategy for the KdV equation

The KdV equation (3.2) consists of a time derivative term and three terms with spatial derivatives. The term η_x can simply be omitted by assuming a moving frame

of reference, since it represents pure translation at constant speed. For the two remaining terms, the linear dispersive term η_{xxx} and the nonlinear term $\eta\eta_x$ different strategies are possible. The main choices are between implicit and explicit methods and the order of the methods. For stability, implicit methods such as the trapezoidal scheme are often preferred, although it means solving a linear system per time step. Explicit methods are cheaper per time step, but this advantage may be outweighed by severe time step constraints. For the linear term in the KdV equation, the trapezoidal rule gives a second order unconditionally stable method without introducing dissipation.

Since the KdV equation contains a nonlinear term, a fully implicit treatment would result in a nonlinear system to solve on each time step. Thus, explicit methods such as the Adams-Bashforth scheme, are more common here. It should also be noted that the nonlinear term may be rewritten as $\eta\eta_x = \frac{1}{2}(\eta^2)_x$ and that the different forms may have different numerical features.

The choice of time-stepping strategy is independent from the spatial discretization method. The implicit-explicit approach sketched out here is applied in combination with a Chebyshev spectral method and a finite difference method in Paper A.

5.3.2 IMPES

Consider the coupled two-phase flow problem in porous media defined by Equations (3.15) and (3.17) with a suitable set of constitutive relations and boundary conditions. The elliptic pressure equation (3.17) is commonly solved implicitly, using saturations, constitutive relations and spatial pressure derivatives from the present time step. This is a natural choice, due to the lack of temporal derivatives in this equation. The elliptic nature of the equation also implies strong global couplings, which are better accounted for using an implicit method. By e.g. including compressibility effects, a time derivative term appears, and the equation takes a parabolic form. However, it is still usually near-elliptic, and an explicit method would require very small time steps due to the CFL criterion.

The hyperbolic saturation equation (3.15), on the other hand, is local of nature, which often allows the use of explicit methods without too severe time step restrictions. The CFL criterion is, however, a function of the maximum velocity in the flow field, which means that for parameter fields with high-permeable flow paths, the restriction may negate the positive effects of avoiding a large linear system solve on each time step. A major advantage of taking shorter time steps is that less numerical diffusion is introduced than with long time steps.

Combining these approaches leads to a sequential scheme where at each time step, the hyperbolic equation is solved explicitly for saturation, and then the saturation values are inputs to the implicit solver for the elliptic equation, which provides pressures. The latter involves a linear system, usually solved by some Krylov method as described in Section 5.2.2. Fluxes are obtained by evaluating Darcy's law, Equation (3.14). This approach is known as the IMPES (IMplicit Pressure, Explicit Saturation) method [47].

5.3.3 Fully implicit method

An alternative approach to IMPES is to solve both equations implicitly. This can be done either sequentially, known as the Sequential implicit method (SEQ) [163,182] or simultaneously, known as the Fully Implicit Method (FIM). The latter is by far the most commonly used in reservoir simulators. In this approach, the nonlinear coupled system is solved implicitly and simulataneously for pressures and saturations. This yields a nonlinear system of equations on each time step, commonly solved using Newton iterations. The resulting Jacobian is a nonsymmetric matrix of dimension $2n \times 2n$.

This method is regarded as unconditionally stable, so long time steps can be taken provided that the Newton iterations converge sufficiently fast. Since the method is significantly more expensive per time step than IMPES, it may not be optimal for cases where the CFL criterion in IMPES is loose. It is also known for introducing numerical diffusion, which may be remedied by shortening the time steps.

An alternative approach combining IMPES and FIM is the Adaptive Implicit Method (AIM), which allows for using FIM in areas where the changes in pressures and saturations are large, and IMPES in other areas [1,168].

In Papers B and C the FIM strategy is applied to two-phase flow in porous media.

5.4 Upscaling

For problems exhibiting features occurring on different scales and it is impossible or impractical to resolve the finest scales, upscaling is a common strategy. This is indeed the case in porous media problems with realistic parameter fields, as well as in many other physical systems. In short, upscaling consists of representing a problem on a coarser resolution than it is originally stated. Upscaling has been subject to intense research effort for the last few decades [44,45,70,144], and covers a wide variety of methods.

Two important properties to consider for two-phase flow in porous media are permeability and saturation. The permeability may for instance change several orders of magnitude over distances far smaller than the attainable grid resolution. Given a fine scale permeability field, a coarse field may be obtained by solving local or global single-phase flow problems and calibrating the results to the coarse grid. Saturations are generally simpler to upscale; this is typically done by taking the average value of the fine scale values over a coarse cell. Coarse scale relative permeabilities and capillary pressures may then be calculated from the coarse saturations.

An underlying concept is the assumption of an equilibrium state with respect to a dominant physical process. For instance, if the time scale is long enough that the phases in a two-phase system separate completely due to gravity, vertically integrated models (VIM) is a natural upscaling [186]. This reduces the dimension of the problem by eliminating the vertical coordinate. If, on the other hand, capillary forces are the dominant cause of saturation heterogeneities, a capillary pressure based upscaling approach is more appropriate, see e.g. [56,143,173]. It is also possible to

include capillary effects such as a fringe, or a smooth transition between the separated phases, in the VIM framework [135].

A demonstration of the importance of upscaling can be found in [127], where vertically integrated models are reported to have CPU times orders of magnitude smaller than full 3D models, while providing results on the same level of accuracy or better.

Upscaling is usually performed on the continuous problem; then the resulting coarse scale problem is discretized and solved. The related class of multiscale methods [23,65,101,107,129] also includes a component for downscaling, or reconstructing the fine-scale solution; this is discussed in the next chapter in the context of preconditioning. An alternative approach to upscaling on the continuous problem, numerical upscaling, consists of first discretizing the fine scale system and then upscaling. This is discussed further in the next chapter and in Paper C in the context of nonlinear preconditioning.

6. Preconditioning

The performance of a linear solver largely depends on the condition number of the coefficient matrix,

$$\kappa(A) = \|A^{-1}\| \, \|A\|. \tag{6.1}$$

A related property is the clustering of the eigenvalues of A. Systems arising from various physical phenomena may often be seriously ill-conditioned, resulting in slow convergence and inefficient solvers. This is true both for the original nonlinear problems and the linearized problems on each Newton step. Preconditioning the system means transforming it to another equivalent, but better conditioned system.

Preconditioning is usually performed on the linear system, and may typically be expressed as a multiplication of the linear system with a matrix M^{-1},

$$M^{-1}Ax = M^{-1}b \tag{6.2}$$

Here, M^{-1} is called a preconditioner. However, the concept of preconditioning is readily generalizable to nonlinear systems [32]. The following section gives an introduction to linear preconditioning. Section 6.2 describes nonlinear preconditioning.

6.1 Linear preconditioning

The ultimate objective of a linear preconditioner is to improve the condition of the system, making it faster to solve using an iterative method. It is readily observed from equation (6.2) that the optimal preconditioner would be $M^{-1} = A^{-1}$, but this would imply solving the problem completely without preconditioner. Hence, a good preconditioner is one that approximates A^{-1} well at a small cost. There are several strategies for achieving this, both by pure algebraic means and by exploiting certain structures in the system. As the linear systems are usually solved by a Krylov method,

the preconditioner is often regarded as a part of the solver. Also, the matrix M^{-1} is often replaced by a function providing the effect of multiplying it with a vector.

Equation (6.2) demonstrates left preconditioning, which is the most common form of preconditioning. An alternative is right preconditioning,

$$AM^{-1}Mx = b, \tag{6.3}$$

which is solved in two steps by solving the systems $AM^{-1}y = b$ and $Mx = y$ for y and x, respectively.

One of the simplest preconditioners is perhaps the Jacobi preconditioner, which is simply constructed by setting $M = \text{diag}(A)$. This works well if A is sufficiently diagonally dominant. Another option is the incomplete LU (ILU) factorization. This is performed by calculating an approximate LU factorization (see Section 5.2.1) and setting $M = LU$. The sparsity pattern is often chosen to equal that of A, this is denoted as ILU(0). By using sparsity patterns of powers of A the accuracy of the approximation may be increased at the cost of execution time. Fill-ins using the sparsity pattern of A^k is denoted by ILU($k-1$).

6.1.1 Domain decomposition methods

Domain Decomposition (DD) methods [146,160,169] is a large class of methods comprising both solvers and preconditioners. As the name suggests, the domain is split into two or more subdomains, and the system is solved in each subdomain using local data on the internal boundaries. A major motivation for DD is parallel computing, as dividing the domain allows for distributing the computations to different processors. Parallel computing is crucial to solving large problems efficiently, and its effect on the DD field is evident from the large activity it has experienced since parallel computers became widely available from the 1980's. However, DD can be traced back to the 19th century [155]. Another motivation that has come up more recently is the development of multiscale methods, which have been shown to have similarities with DD [133].

Before moving on with the presentation of DD methods, it is useful to define two operators, namely the compression operator $\mathcal{C}$ and the reconstruction operator $\mathcal{R}$ [62,134]. The compression takes a global fine scale property as input, and outputs a coarse or localized property. Subscripts are used to distinguish different operators. These operators should satisfy the relation

$$\mathcal{C}\mathcal{R} = \mathcal{I}, \tag{6.4}$$

that is, reconstructing a coarse or local property and then compressing it back to the should give the starting value. On the other hand, in general we have $\mathcal{R}\mathcal{C} \neq \mathcal{I}$, since information lost in the compression operation cannot be reconstructed. These operators are in general nonlinear. In cases where linear operators are assumed, a normal typeface is used.

Since the cost of iterative solvers typically scales with $O(n^2)$, solving several smaller problems once may be significantly cheaper than solving the whole problem. However, solving the smaller problems only once would not suffice due to the lack of global information, so an iterative procedure or a global coarse level solver is required. When DD is applied as a stand-alone linear solver, both iterations and a coarse level is needed. The most usual situation, however, is using DD as a preconditioner, since as a solver it is generally slow compared to alternatives such as Krylov methods. The coarse level is particularly important for elliptic problems with strong global couplings, as each subdomain only interacts with its immediate neighbours. The terms one-level and two-level DD refers to DD methods without and with a coarse level, respectively. A major divide between different DD methods is between overlapping and non-overlapping methods [19]. Overlapping methods are typically known as Schwarz methods and nonoverlapping methods as substructuring methods [18]. We will confine this presentation to Schwarz methods.

The alternating Schwarz method was developed by H. A. Schwarz as a theoretical tool for solving partial differential equations on domains consisting of a finite number of overlapping subdomains almost one and a half century ago [155]. The convergence was proved in the 1950's [123], but the interest first took off in the 1980's [10] with

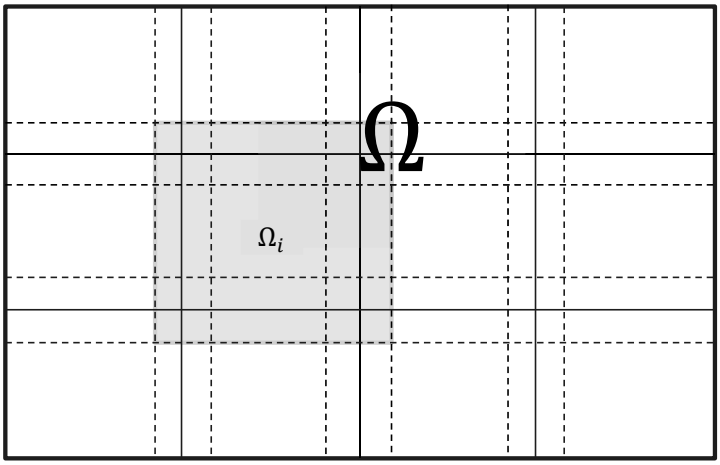

Figure 6.1: A non-overlapping (continuous lines) and an overlapping (dashed lines) decomposition of a rectangular domain Ω. A subdomain Ω_i in the overlapping decomposition is indicated by the shaded area. In general, the domains and subdomains may have arbitrary shapes.

the advent of parallel computing. In Figure 6.1 a conceptual sketch of an overlapping DD partitioning is shown.

The most well-known Schwarz algorithms are the Additive Schwarz (AS) [61] and the Multiplicative Schwarz (MS) [21] methods. The one-level AS method can be written out as an iterative method as

$$x_{\Omega_i}^{(k+1)} = x_{\Omega_i}^{(k)} + A_{\Omega_i}^{-1}\left(b_{\Omega_i} - A_{\Omega_i}x_{\Omega_i}^{(k)} - A_{\Omega\setminus\Omega_i}x_{\Omega\setminus\Omega_i}^{(k)}\right), \quad i = 1, \dots, n_p \tag{6.5}$$

where $\Omega_i \subset \Omega$ are the n_p overlapping subdomains and used as a subscript indicates that only the rows and columns corresponding to this subdomain are included. The local coefficient matrix is defined by

$$A_{\Omega_i} = C_{\Omega_i} A R_{\Omega_i}, \tag{6.6}$$

where the compression operator C_{Ω_i} is simply a restriction matrix from Ω to Ω_i. Normally, the reconstruction satisfies $R_{\Omega_i} = C_{\Omega_i}^T$. The $\Omega\setminus\Omega_i$ term represents local boundary conditions. This notation strictly denotes the whole of the domain except

Ω_i, but in practice only values near the boundary of the subdomain are involved. As indicated by the inverted local matrix in the formula, a local version of the linear system is solved on each subdomain on each iteration step. AS is seldom used as a stand-alone solver like in equation (6.5), as this method converges rather slowly. Rather, it is used as a preconditioner for the linear system. This corresponds to performing one iteration using formula (6.5), and then combining the results to a single preconditioning matrix, e.g.

$$P_{AS} = \sum_{i=1}^{n_p} R_{\Omega_i} A_{\Omega_i}^{-1} C_{\Omega_i}. \tag{6.7}$$

In practice, a matrix on this form is not constructed explicitly, but the effect of multiplying it with a vector, typically on the form $y = Av$, is obtained from a function performing local solves and combining the results. When used in conjunction with a Krylov solver for linear problems arising from a Newton iteration, the resulting overall algorithm is known as a Newton-Krylov-Schwarz (NKS) method [10,31].

For problems with strong global couplings, such as the (near-)elliptic pressure equation often encountered in porous media problems, the one-level strategy has a major flaw in that the couplings, represented by the $\Omega \backslash \Omega_i$ term in Equation (6.7), are localized. Each subdomain only has direct access to information from its immediate neighbors, with the result that a signal needs at least as many iterations as there are subdomains in-between to travel from one subdomain to another. In massively parallel implementations, this becomes a serious problem, as scalability with respect to the number of subdomains is essential there. The solution is to add a coarse level, which acts as a global subdomain, typically with the local subdomains as coarse grid cells. This extension from a one-level to a two-level method is rather straightforward by denoting the coarse level by index 0 and starting the counter i in equations (6.5) and (6.7) from 0 instead of 1. Scalability issues for linear AS are addressed in Paper B.

AS is similar to the Jacobi method in the sense that it only uses information from the previous iteration step. Hence, it can be fully parallellized straight away. In fact, it can be seen as an overlapping version of the block Jacobi preconditioner [13]. Similarly, MS can be seen as an overlapping Gauss-Seidel preconditioner, using the most recent available information and thus needing a subdomain coloring strategy in order to be parallelizable.

When it comes to handling the overlaps, there are several strategies available. After solving all the local problems (6.5) once, there are several local problem solutions that need to be unified to form the preconditioned global problem, and in the overlapping regions there are multiple solutions that are generally different. The simplest option is to simply add the overlapping solutions, giving the formula (6.7), however, this will yield non-physical solutions in the overlap. A better option is to weight the sum using some partition of unity, e.g. by taking the arithmetic average of the solutions. The RAS (restricted AS) and ASH (AS with harmonic extension) [36] methods takes a different approach by replacing $R_{\Omega_i}^T$ (RAS) or R_{Ω_i} (ASH), respectively, in formula (6.7) by the non-overlapping equivalents. A further improvement of these methods is found in the RASHO (Restricted AS with Harmonic Overlap) method [29].

The theory behind AS and other domain decomposition methods is largely developed with symmetric positive definite elliptic problems in mind, such as single-phase flow in porous media. For two-phase flow, coupled elliptic-hyperbolic problems arise, and the hyperbolic part may need a different treatment [185]. Due to the local nature, the concerns about scaling with respect to number of subdomains are rather small. However, the overlaps could be better handled by incorporating information from the local flow field. By determining which subdomain is most upstream, one can choose to use this subdomain solution in the global solution and discard the solution from the more downstream subdomain. This makes sense physically as the domain of dependence of a purely hyperbolic equation is contained in the upstream part of the domain. It should be noted that for complex flow patterns e.g. due to heterogeneous parameter fields the upstream direction for an overlap region is not always uniquely

determined, so some heuristics are needed, but in total this should give a more physically sound overlap handling than e.g. averaging.

The shape of the subdomains and coarse grid cells may have a large impact on the results. While e.g. rectangular subdomains may be convenient from a proof-of-concept point of view, an optimal partitioning is one that honors the parameter field e.g. by seeking to avoid discontinuities in the parameters inside the subdomains [154].

6.1.2 Multigrid and multiscale preconditioners

Multigrid methods (MG) [81] are a class of methods that are based on the use of multiple grids with varying resolution to handle errors of different frequencies. As DD, they can be applied as stand-alone solvers or as preconditioners [13]. As solvers they are typically used together with a stationary iterative method such as Jacobi, Gauss-Seidel or SOR. Multigrid methods may be classified as geometric (GMG) or algebraic (AMG) [25,69,165]. AMG provides a method based solely on the coefficient matrix, not on the geometry of the system, and has proven to be well-suited as a preconditioner for e.g. multiphase flow problems in porous media [166]. Another preconditioner highly relevant for fully implicit simulations of multiphase flow in porous media is the Constrained Pressure Residual (CPR) method [178], which directly addresses the mixed nature of these problems. CPR may also be used in combination with AMG for fully implicit simulations [38]. Both AMG and CPR are two-stage preconditioners, with different techniques applied on the different stages.

A class of preconditioners that is related to the upscaling concepts introduced in Section 5.4 is the multiscale preconditioners. While the term 'multiscale' is not uniquely defined, a distinguishing feature may be that while upscaling methods can provide a coarse scale representation of a problem, multiscale methods also has a downscaling component that allows for reconstructing the fine scale solution. This makes MSM a natural candidate for a preconditioner for problems where resolving all the involved scales directly is infeasible. This is the case for many different realistic

physical systems, including flow in porous media. A large variety of methods based on different equation formulations and discretizations have been developed, e.g. the Variational Multiscale Method (VMS) [89–91,100], the Multiscale Finite Element Method (MFEM) [85,86], the Multiscale Finite Volume method [97,98,189], Multiscale Mortar Mixed Finite Element Method [9] and the Heterogeneous Multiscale Method (HMM) [62] to name a few.

These methods may be used as preconditioners for the linear system arising from a discretized single-phase flow problem. It has been shown that some of these methods are similar to, and in special cases equivalent to, DD methods [76,130,133,153].

As an example of the relation between upscaling and multiscale methods, consider the vertically integrated models introduced in Section 5.4. While the upscaled model only solves the two-dimensional compressed coarse problem, it can be extended to a multiscale method by introducing a reconstruction $\mathcal{R}$ from the coarse scale to the three-dimensional fine scale. The key of a successful reconstruction is then to have an intuition about the physical distribution of properties in the vertical dimension.

When reconstructing the fine scale saturation profile, the simplest option is to have a constant value corresponding to the coarse saturation along the vertical direction. This is non-physical as long as the assumption of gravitational equilibrium that VIM relies on is met. If a sharp interface is assumed, a reconstruction operator that distributes the fluid phases with all of the light fluid on top of the heavy fluid is employed. If a capillary fringe is assumed, a smoother transition taking capillary effects into account is applied [134]. These variations in assumed fine-scale structure can be expressed through the reconstruction operator alone.

6.2 Nonlinear preconditioning

While the preconditioning methods presented above work on and in some cases exploit features of the linearized system, the system that ultimately is of interest is the original nonlinear problem. The preconditioning efforts on each nonlinear iteration

step can at best increase the efficiency of that step, but not reduce the number of steps needed.

Further, much of the underlying physics are lost in the linearization process. It may sometimes be desirable to work directly on the original nonlinear set of equations in order to take advantage of some of the physical features of the problem. In order to achieve this, different approaches may be taken. In this section we will emphasize an approach based on nonlinear domain decomposition (NLDD), which is also studied in Papers B, C and D.

6.2.1 Nonlinear domain decomposition methods

Nonlinear preconditioning aims to improve the condition of a nonlinear problem. A poorly conditioned problem is characterized by unbalanced nonlinearities between the different components of the problem, and the preconditioner seeks to transform the problem to an equivalent one with more balanced nonlinearities. Note that the term 'nonlinear preconditioning' may also be used to describe strategies for linear systems where the preconditioner itself is nonlinear, i.e. it cannot be expressed as a matrix M^{-1}, see e.g. [41]. Here, we use the term for preconditioning of nonlinear problems.

A DD based framework for nonlinear preconditioning, the Additive Schwarz Preconditioned Inexact Newton (ASPIN) method was proposed by Cai and Keyes [32], and has been used in diverse applications such as computational fluid dynamics [32,34,92,93], image processing [190] and optimization problems related to nonlinear elasticity [77]. ASPIN is based on the nonlinear AS method [30,60] and the inexact Newton method [54]. The principle behind nonlinear AS is the same as for the standard linear version; the difference lies in that it is applied on a nonlinear problem instead of a linear problem. The following presentation is largely based on [7,32]. Given a generic nonlinear problem,

$$F(u) = 0, \qquad u \in \Omega, \tag{6.8}$$

ASPIN defines an equivalent preconditioned problem

$$\mathcal{F}(u) = 0, \tag{6.9}$$

where $\mathcal{F}(u)$ is obtained by solving local nonlinear problems on the form

$$F_i(u - \delta_i(u)) = 0, \quad i = 1, \dots, n_p \tag{6.10}$$

The δ_i's are the local updates to the global state u, and the nonlinearly preconditioned residual is defined as

$$\mathcal{F}^{(1)}(u) = \sum_{i=1}^{n_p} \delta_i(u). \tag{6.11}$$

Here, the superscript indicates that this is a one-level preconditioner. After solving n_p local nonlinear problems, a global, nonlinearly preconditioned Newton iteration step is performed by solving the linear system

$$\mathcal{J}^{(1)}\big(u^{(k)}\big)\Delta u^{(k)} = -\mathcal{F}^{(1)}\big(u^{(k)}\big), \tag{6.12}$$

where $\mathcal{J}^{(1)}$ is the Jacobian of the nonlinear residual, defined as

$$\mathcal{J}^{(1)}(u) = \sum_{i=1}^{n_p} \delta_i'(u), \tag{6.13}$$

and

$$\delta_i'(u) = R_i\big(C_i J\big(u - \delta_i(u)\big)R_i\big)^{-1} C_i J\big(u - \delta_i(u)\big). \tag{6.14}$$

From a computational perspective, it is undesirable to evaluate this formula exactly, so the approximation

$$\tilde{\delta}_i'(u) = R_i(C_i J(u) R_i)^{-1} C_i J(u) \tag{6.15}$$

is commonly done. This is based on assuming u to be close to the true solution, in which case the updates δ_i are small [7,32]. The Jacobian is then expressed as $\tilde{\mathcal{J}}^{(1)}(u) = \sum_{i=1}^{n_p} \tilde{\delta}_i'(u)$, and the global linear problem is solved by an inexact Newton

method. This typically includes a post-processing step using a globalization technique such as linesearch [55,128], which has the effect of shortening the Newton step and improving the convergence. The linear solver is usually a Krylov solver, e.g. GMRES [149,177].

The resulting algorithm consists of three levels of iterative methods; Global newton iteration (outermost), local Newton iterations for constructing the preconditioner, and a Krylov linear solver for solving the resulting global Jacobian system (innermost). For the local Newton iterations it may, depending on subdomain size, be reasonable to use a direct solver. This method resembles the standard NKS methods in the sense that the same building blocks are involved, with the main difference in how the Schwarz component is applied. Also, the approximate version of the Jacobian, $\tilde{J}^{(1)}(u)$, is exactly the same as the exact preconditioned Jacobian in the corresponding NKS method, which is beneficial from an implementational point of view.

A two-level version of ASPIN was introduced in [33]. We will briefly outline the preconditioner presented there in the following. The coarse and fine scale problems are assumed to approximate each other in some sense, and the coarse scale solution u_0^* is assumed to be known or easily obtainable through pre-processing. The fine scale components of the two-scale preconditioner equal the one-level preconditioner presented above. The construction of the coarse scale component is somewhat more complex. Let $T^C(u)$ be defined as the solution of the coarse nonlinear system

$$F_0\big(T^C(u)\big) = C_0 F(u), \tag{6.16}$$

where C_0 is the compression, or restriction, operator from fine to coarse scale. This may be interpreted as finding the coarse scale solution that gives the same coarse residual as the compressed fine scale residual of the fine scale solution u. It is readily observed that by inserting the true fine scale solution $u = u^*$, we can write

$$F_0(u_C^*) = C_0 F(u^*), \tag{6.17}$$

that is, $T^C(u^*) = u_C^*$. By letting $T_0(u) = R_0 T^C(u)$, where R_0 is the reconstruction, or prolongation, operator from coarse to fine scale, we can write $T_0(u^*) = R_0 u_C^*$. The preconditioned system is then defined as

$$\mathcal{F}^{(2)}(u) = 0, \tag{6.18}$$

where

$$\mathcal{F}^{(2)}(u) = T_0(u) - T_0(u^*) + \mathcal{F}^{(1)}(u). \tag{6.19}$$

For the Jacobian, $\mathcal{J}^{(2)}(u)$, the same type of approximation as on the fine scale is typically used. Following the presentation of [33], problem (6.18) is solved with some $u^{(0)}$ as the initial guess. An modified approach, which rather uses $T_0(u^*)$ as the initial guess has been reported to perform better [111]. This implies a multiplicative relation between the coarse and fine levels. A different approach is to use a linear coarse solver. This was introduced in [92] motivated by computational savings from not having to solve a nonlinear coarse system. The robustness and scalability properties of the method were reported to be similar to the nonlinear coarse scale approach.

A convergence proof of one-level ASPIN was given by An [7]. A multiplicative variant of one-level ASPIN (MSPIN) is presented in [67].

The nonlinear approach to preconditioning presented above has several interesting implications. One is that if the nonlinearities are localized to small parts of the domain, the computational effort is automatically localized to these regions, as subdomains with high degree of nonlinearity will require more Newton iterations than subdomains with low degree of nonlinearity. A consequence of this is that otherwise wasted operations (as in a global approach) are saved, but in order to utilize these savings, load balancing must be carefully considered, e.g. by designing the partition such that the presumably most demanding subdomains are smaller than less demanding ones [32].

Different aspects of ASPIN are treated in Papers B, C and D, with the two former considering two-phase flow in porous media, and the latter nonlinear elasticity. In Paper C ASPIN is suggested as the basis for physics-based preconditioners, linking numerical upscaling and preconditioning.

6.2.2 Other approaches

Other nonlinear DD methods include the nonlinear FETI (Finite Element Tearing and Interconnect) method [108,138], which belongs to the class of substructuring methods. An approach that is related to ASPIN is the nonlinear elimination method [35,94,95,180], which seeks to reduce the components in the residual vector with the highest magnitude in order to obtain a more well-balanced system with respect to nonlinearities. The nonlinear multigrid approach known as the Full Approximation Scheme (FAS) has been around for several decades [22,24,181] and has been widely used for several application fields.

Reordering methods and methods for adaptive localization of Newton iterations have also been applied with success in the context of multiphase flow in porous media [8,113,126,187]. This type of methods could possibly be combined with ASPIN to further enhance performance.

7. Summary of papers

Paper A

A boundary value problem for the KdV equation: Comparison of finite-difference and Chebyshev methods

Jan Ole Skogestad and Henrik Kalisch

Published in *Mathematics and Computers in Simulation*, Vol 80 (1), pages 151-163, 2009

In this paper a comparison of two different spatial discretization methods for the Korteweg-de Vries equation is performed. A finite difference scheme, as presented in Section 4.1.1 and a spectral method based on Chebyshev polynomials, as presented in Section 4.1.2.

Fourier-based spectral collocation methods have long been popular for the KdV equation, much due to the Fast Fourier Transform (FFT). These methods use trigonometric interpolating polynomials, and require periodic boundary conditions. For cases where periodic boundary conditions are not suitable, such as in studies of undular bores, other methods are required. One option is to turn to finite difference methods, but there also exists spectral collocation methods capable of handling non-periodic boundary conditions. Methods using polynomial interpolating functions, such as Chebyshev polynomials, fall into this class, but have received less attention than Fourier methods and thus need more research. While the convergence rates are excellent, the Chebyshev methods some unattractive features, such as clustering of grid points near the boundaries of the domain and, as with Fourier methods, dense coefficient matrices.

The major goal of this paper is to examine a Chebyshev spectral method and a finite difference method in order to determine which is the better choice of discretization

strategy in terms of computational performance for a boundary value problem for the standard KdV equation.

The problem is set up with a homogeneous Dirichlet condition in each end of the finite domain and a homogeneous Neumann condition at the rightmost end. The initial condition is a single soliton. The time integration is performed by a combination of the implicit Crank-Nicholson (for the third order term) and the explicit Adams-Bashforth schemes, both of second order. Stability properties for the methods are discussed, and while it is noted that the time integration scheme is in principle unstable, the growth factor approaches 1 rapidly as the time step tends to zero.

The main result is that the Chebyshev spectral method performs better, although it may face some stability challenges for grids of high resolution, since this will yield very small local grid sizes near the boundaries.

Paper B

Domain decomposition strategies for nonlinear flow problems in porous media

Jan Ole Skogestad, Eirik Keilegavlen and Jan M. Nordbotten

Published in *Journal of Computational Physics*, Vol 234, Pages 439-451, 2013

In this paper we study different strategies for applying domain decomposition to a non-linear flow problem in a porous medium. Specifically, the one-level Additive Schwarz (AS) method is presented as a solver and a preconditioner, applicable to linear or nonlinear problems. This gives four different options on how to apply AS to a nonlinear problem.

The model problem is a coupled elliptic-hyperbolic problem describing flow in porous media. By varying parameters such as permeability and porosity, mobilities and viscosity ratios, a suite of seven different problems ranging from completely linear on a homogeneous domain to severly nonlinear on a challenging heterogeneous permeability field are obtained. The different AS approaches are then compared for fully implicit simulations the different problems.

As excpected, preconditioners outperform solvers, both in the linear and nonlinear case. For the linear case this is already established in the literature, while for the nonlinear case such a comparison has to the authors' knowledge not been done before for flows in porous media. Further, the nonlinear preconditioner (ASPIN, see Section 6.2.1), is shown to perform up to 75 % better than the linear counterpart.

Scalability and sensitivity to simulation parameters is also discussed. It is evident that a coarse component is needed to account for the global couplings in the elliptic part of the problem both for the nonlinear and the linear preconditioners in order to reduce scaling effects.

Paper C

Two-scale Preconditioning for Two-phase Nonlinear Flows in Porous Media

Jan Ole Skogestad, Eirik Keilegavlen and Jan M. Nordbotten

Submitted to *Transport in Porous Media*

This paper presents a new framework for two-scale preconditioning allowing for input of physical intuition from the user. The work here is based partly on the foundation that was laid in Paper B, where one-level ASPIN [32] was found to be a competitive preconditioner for two-phase flow in porous media, and partly on previous work on two-level ASPIN preconditioners [33,92,93,121].

The underlying idea of the paper is to provide a framework for bridging the gap between upscaling and solvers and validate its applicability as a precondtioner for coupled nonlinear two-phase flow problems in porous media by studying the scalability properties of the method.

The proposed framework can be seen as a generalized version of the previously established two-level ASPIN. In previous work on two-level ASPIN, there has not been given much attention to the operators between the coarse and fine spaces. These operators, and especially the reconstruction operator from the coarse to the fine level, are at the core of the new framework. The reconstruction operator is allowed to be nonlinear, and it takes the previous fine scale state as an input, in addition to the coarse scale update. The latter point is important; the coarse solver only solves for updates to a given fine scale state, there are no explicitly represented coarse, or upscaled, variables such as pressures and saturations. The continuous model is entirely given on the fine scale.

By exploiting the flexibility in the reconstruction operators, however, something reminiscent of a numerical upscaling is achieved. If a dominating physical process can be assumed, a reconstruction operator based on this assumption may be formed

and in the limiting case the coarse solver will, theoretically, produce a solution that is valid on the fine scale. The computational complexity in this case will in theory be similar to that of solving an upscaled problem as only coarse problems are solved. On moving away from the limit, the upscaling assumption becomes increasingly invalid, but this framework still provides an efficient solution strategy by using the coarse solves as a part of a two-level ASPIN-type preconditioner for the non-linear system.

In order to establish this framework, we study the behavior of the method in its most simple form, that is, we use a standard linear reconstruction operator. For validation purposes, weak and strong scalability is studied. The method is found to improve greatly on the one-level ASPIN method, obtaining a performance virtually independent on the number of subdomains.

An exception is cases with strongly channelized permeability fields, where the performance improves relative to the one-level method, but still depends on the number of subdomains. This may be explained by a non-optimal partition strategy, which in our tests is based on dividing the domain in uniformly sized rectangular subdomains. A strategy based on honoring the structure of the parameter field might likely produce better scalability results for these permeability fields.

The conclusion of this study is that a two-scale preconditioning strategy with the potential of bridging upscaling and solvers, has been validated, thus forming a foundation for further studies of physics-based preconditioners.

Paper D

Domain decomposition preconditioning for non-linear elasticity problems

Eirik Keilegavlen, Jan Ole Skogestad and Jan M. Nordbotten

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In this paper one- and two-level ASPIN strategies is applied to nonlinear elasticity problems. Scalability with respect to linear and nonlinear iterations is studied for problems with homogeneous and heterogeneous parameter fields. Furthermore, together with Papers B and C, this paper also shows the independence of underlying discretization methods, as here, a finite element method is used, in contrast to the control volume and upstream differencing methods used in the other papers.

The performances of one- and two-level ASPIN and a two-level linear DD strategy are compared for two different parameter fields, a homogeneous and a heterogeneous field. The heterogeneities consist of circular inclusions in an otherwise homogenous field, a choice made in order to explore effects of local nonlinearities.

For the homogeneous problem, the two-level methods are found to scale well. The one-level ASPIN method, on the other hand, scales poorly. This is expected from DD theory, and is in line with the findings in Paper B. The local boundary conditions become inaccurate due to the lack of a coarse solver to handle the global nature of the problem.

The effect of material heterogeneities is studied by varying the contrast in coefficients between the inclusion and the surrounding area. It turns out that for high contrasts, the one-level method performs better than the two-level method in terms of global and local nonlinear iterations, while the two-level method is consistently better in terms of linear iterations. The explanation of the comparatively weak nonlinear performance of the two-level method is suggested to be that the residual is confined

to the edge of the inclusions within each subdomain, and thus not resolvable by the coarse solver. Since the coarse scale operators do not adapt to the fine scale state, the initial guess to the local fine scale solves becomes poorer than for the one-level ASPIN method.

8. Conclusions and further work

This work is a study of mathematical problems arising from nonlinear conservation laws in different physical settings, with focus on the solution strategies.

For the KdV equation, which is well-known as a model for surface gravity waves, a spectral collocation method based on Chebyshev polynomials, which have been shown relatively little attention previously, has in Paper A been shown to be a strong competitor against other discretization strategies, specifically finite difference methods. The Chebyshev method performs better in terms of execution time as both the spatial grid and the time steps are refined.

Due to the special structure of this equation, the standard procedure of linearizing through Newton iterations can be avoided as the nonlinearity is confined to one term that relatively easily may be discretized explicitly.

In the case of multiphase flow in porous media, the complexity is higher, both in terms of couplings between different processes, nonlinear constitutive relations and multiscale phenomena. On top of this, the data describing the porous medium are highly uncertain. These challenges have spawned a large research effort in order to solve problems related to porous media flow faster and in a more robust manner. This includes preconditioners, linear solvers, upscaling and multiscale methods. A common approach is to handle the nonlinearities through a Newton iteration, and then focusing on solving the resulting linear systems more efficiently.

A suggestion for future work is to put focus on solving the original nonlinear problem in a best possible manner, and incorporate physical information in solvers and preconditioners. A useful foundation for this has been found in the nonlinear preconditioning framework of ASPIN [32]. We have in Papers B and C demonstrated that this framework is well-suited and scalable for nonlinear porous media flows. In Paper C we also suggest modifications on the method in order to better account for the multiscale nature of these problems, in a way that bridges together nonlinear preconditioning and upscaling. In theory, this should result in a numerical upscaling

method in the equilibrium limit. This should fall out automatically as this limit is approached, in what might be called automatic upscaling. In order to establish this numerical upscaling framework, further work is needed in order to demonstrate the behavior of the method as the upscaling limit is approached for relevant cases, in addition to analysis and benchmarking against other methods.

In order for the automatic numerical upscaling to work, the compression and reconstruction operators should be designed such that they mimic the behavior of the analytical upscaling process and honor the fine scale structure of the system. This is achieved by considering energy minimization, or assuming equilibrium, with respect to a dominating physical process. Then, if the assumptions are met, the reconstructed fine scale solution from the coarse update will be converged. Otherwise, the coarse solver acts as a component in a two-level ASPIN preconditioner, whose performance likely depends highly on how far from equilibrium the state actually is. This requires that the user has at least some intuition about the nature of these processes.

The proposed framework has some similarities to the analytical VIM method presented in [78], where the vertical equilibrium assumption is relaxed by dynamically reconstructing pressures and saturations in order to increase the applicability range of VIM.

A feature distinguishing our approach from regular upscaling, is that no coarse scale equations, nor coarse variables, need to be defined. The system is described using fine scale equations and variables, with the compression and reconstruction operators forming a coarse system, which is solved for coarse updates to the current fine scale state. Hence, coarse variables such as pressures and saturations are never calculated.

Finally, one- and two-level ASPIN is demonstrated for nonlinear equilibrium problems in elasticity, showcasing the effect of local nonlinearities within subdomains and how a coarse operator should be used with care, as it may actually worsen the performance compared with a one-level method. Apart from this, scalability results are as expected both for linear and nonlinear iterations. The key to

success lies in careful design of the reconstruction operator, using knowledge about the fine scale structure of the system.

It is important to keep in mind that while the models in Papers B-D are simplified with respect to realistic applications, the methods presented are derived for general equation forms.

For the studies related to nonlinear preconditioning, further work includes analysis of the methods, investigations of the parallel performance of the methods with special focus on load balancing and simulations on realistic 3D reservoir models and more advanced elasticity problems. Another direction is the application of the ideas from Paper C to other physical systems. The stopping conditions for the inexact Newton iterations has not been a major focus in this study, but may be further investigated in order to optimize performance. For an a posteriori error estimation based framework for finding stopping criteria, see e.g. [66,174].

ASPIN has been held up as a candidate strategy for extreme-scale [28,104] and multiphysics [105] simulations, together with other nonlinear strategies such as FAS, nonlinear elimination, and others. This is also relevant in the case of flow in porous media, and it is natural to consider ASPIN-based strategies in light of other available nonlinear strategies.

For the KdV equation, further work may include comparison of the Chebyshev based collocation method with other methods, e.g. the hybrid Legendre-Petrov-Galerkin and Chebyshev method by Ma and Sun [120], and similar comparisons for other equations in the KdV family.

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