Introduction

The present thesis deals with the efficient adaptive numerical integration of dynamical contact problems. This is the core problem in the fast and robust simulation of stresses arising in a real patient's knee joint for different kinds of loading situations. The topic is of high interest in the field of *computer-assisted therapy planning*, which aims at the generation of a "virtual patient" [17]. This tool allows the design of effective treatment options and precise surgery strategies within a clinical environment. Potential tasks of patient-specific techniques in orthopedics are osteotomic interventions and the construction and selection of implants or fixation devices.

For realistic predictions of therapeutical manipulations, numerical simulation and optimization are applied on a detailed three-dimensional geometry of the individual patient's knee (obtained from anatomical CT or MRT image data). In view of a reasonable clinical application, the necessary computations have to be performed on local workstations in clinics within short time frames. Moreover, the solutions have to be resilient enough to serve as a basis for responsible medical decisions. With regard to these conditions, highest level requirements have to be set on the efficiency and accuracy of the applied numerical techniques.

The appropriate approach to cope with this mathematical challenge is the construction of an adaptive numerical integrator for the dynamical contact problem. For this purpose, dynamical contact problems have to be analyzed precisely from both the analytical and the numerical point of view.

Dynamical Contact Problems. In 1933, Antonio Signorini introduced the frictionless static contact problem of a linearly elastic body with a rigid foundation [85], which today is called Signorini problem. Since then, the modeling of contact phenomena classically employs Signorini's contact conditions in displacements, which are based on a linearization of the physically meaningful non-penetrability of masses.

Following the same approach in the time-dependent case leads to highly nonlinear second-order variational problems, where the actual zone of contact is a priori unknown. When the phase of contact changes, shocks are caused, which identify the hyperbolic structure of the problem. This inhibits general regularity of an evolution, even if the rest of the data are smooth. Partial regularity results and some discussion on the subject have been published in [13, 23, 68].

For dynamical contact problems between a linearly elastic body and a rigid foundation that are formulated via Signorini's contact conditions, the first existence and uniqueness results were obtained by Duvaut and Lions [23]. They studied problems with prescribed time-constant normal stresses where the contact surface is known in advance. However, up to date, existence results have only been provided for special cases such as some simple geometric settings and one-dimensional problems [68,83]. A general existence or even uniqueness theory in conjunction with pure linear elasticity is still missing.

The serious mathematical problems encountered in proving well-posedness basically originate from the discontinuity of the velocities at contact. The assumption of viscous material behavior allows at least the derivation of existence results for unilateral dynamic contact problems: Jarušek analyzed a frictionless viscoelastic body with singular memory [42,44]. Viscoelastic materials satisfying a Kelvin-Voigt constitutive law were studied by Kuttler and Shillor [62] and Cocou [13]. Kuttler and Shillor proved existence for the case of frictional contact and a moving rigid foundation, while Cocou considered a problem with nonlocal friction. Migòrski and Ochal investigated a class of problems modeled by hemi-variational inequalities [74]. In 2008, Ahn and Stewart established existence for frictionless dynamical contact problems between a linearly viscoelastic body of Kelvin-Voigt type and a rigid obstacle [6]. A survey of existence and uniqueness results is given in the monograph [25] by Eck, Jarušek, and Krebeč.

The papers cited above primarily concern existence results for dynamical contact problems. Uniqueness and continuous dependence on the initial data have not been proven up to now, neither in the purely elastic nor in the viscoelastic case. The fundamental mathematical difficulties with such results can be traced back to the intrinsic non-smoothness of the problem emerging from Signorini's contact conditions. For this reason, the requirement of exact non-penetration of the bodies is often relaxed by using regularization techniques in the analytical models. However, for the medical applications discussed above, any violation of the contact constraints is unacceptable.

Numerical Integration. Over the last decades, a large amount of work has been done on the design of numerical methods for solving dynamical contact problems, which is and remains a challenging task. An overview on several known time discretization schemes can be found, e.g., in the monograph [65] or in the papers [22,59]. Among them, the *classical Newmark method* is one of the most popular numerical solvers, which is also used in the wide-spread finite element analysis program NASTRAN. Unfortunately, it is well-known that this scheme may lead to an unphysical energy blow-up during time integration and numerical instabilities at dynamical contact boundaries may occur. For this reason, Kane, Repetto, Ortiz, and Marsden introduced a *contact–implicit* version which is energy dissipative in contact, but still unable to suppress the undesirable oscillations [46]. Recently, Deuflhard, Krause, and Ertel proposed a *contact–stabilized* variant, which avoids the unphysical oscillations at contact interfaces and is still energy dissipative [19]. For related stabilizations see [87, 88].

Laursen, Chawla, and Love have designed time integration schemes of Newmark type with predominant focus on energy conservation of the discretized solution [66, 67]. Such approaches typically lead to possible interpenetration originating from a discretized persistency condition. However, the biomedical applications in mind require strict non-penetration. For the same reason, enforcement with penalty methods or enforcement with contact conditions in velocities are ruled out.

A different approach for reducing artificial oscillations at contact boundaries has recently been suggested by Khenous, Laborde, and Renard [47, 48]. Their mass redistribution method is based on completely removing the mass in a small strip on the contact boundaries. The algorithm has been further improved by Hager, Hüeber, and Wohlmuth in view of computational cost [31]. However, the scheme is formulated within the method of lines framework, which in general inhibits the development of efficient adaptivity in space. In contrast, the contact–stabilization by Deuflhard et al. leaves the mass matrix unchanged and can easily be applied for arbitrary spatial discretization.

In the absence of contact, any symmetric variant of Newmark's method is equivalent to the Störmer-Verlet scheme, which is well-known to be second-order consistent and convergent (see, e.g., the textbook [33] of Hairer, Lubich, and Wanner). In the presence of contact, the question of consistency and convergence has not been solved yet for any of the discretization schemes presented above. This is due the high irregularities encountered at contact interfaces in the constrained problem, which inhibit the derivation of viable estimates for the local discretization errors via the classical approach.

Adaptivity. The efficient and reliable simulation of the motion of a human knee joint requires a stable numerical integrator for dynamical contact problems, which allows for adaptivity both in time and in space. An equidistant mesh can not be expected to be adequate for reaching a given accuracy of the approximation with a reasonable computational effort. However, until now, the topic of an adaptive timestep control for discretizations of dynamical contact problems has completely been avoided both in engineering and in mathematical literature. This is mainly due to the lack of perturbation and consistency results in the constrained situation.

The present thesis will work out an efficient adaptive time integrator for frictionless dynamical contact problems in viscoelasticity that are formulated on the basis of Signorini's contact conditions. Apart from medical treatment planning, the issue is of wide need in many different application areas such as structural mechanics or metal forming processes.

Outline

Chapter 1 will deal with the mathematical model used to describe frictionless dynamical contact between two viscoelastic bodies fulfilling the Kelvin-Voigt material law. Both the strong and weak problem formulation are presented, which are based on Signorini's contact conditions for bilateral contact. Moreover, conservation properties and the validity of a persistency condition will be discussed. *Chapter 2* will be devoted to the numerical integration of dynamical contact problems. Here, a detailed theoretical and numerical analysis of the classical, the contact–implicit, and the contact–stabilized Newmark method will be given. The presentation will motivate the development of an improved contact–stabilized version, which is the time discretization scheme of interest in this thesis.

In a first step towards an adaptive timestep control, a norm in function space has to be determined in which a perturbation result is satisfied even in the presence of contact. By reason of the present unclear situation in view of well-posedness of dynamical contact problems, *Chapter 3* will concentrate on a stability study under perturbations of the initial data for both the elastic and the viscoelastic case. This will necessitate the definition and interpretation of a stability condition that characterizes a suitable class of contact problems. In a second step, the construction of an adaptive timestep control requires the derivation of a consistency result and the corresponding consistency order. In order to fill the lack of such knowledge for Newmark methods under contact constraints, *Chapter 4* starts with an investigation of the Newmark schemes in function space. Then, consistency error estimates will be derived in the specific norm found in the earlier perturbation theory and in a further discrete norm. Moreover, the consistency behavior of the Newmark methods in the special case of permanent active contact will be analyzed. Subsequently, a novel proof technique will be introduced in *Chapter 5*, which allows showing convergence of the improved contact–stabilized Newmark methods in both norms. This requires in particular the derivation of perturbation results for the scheme, which are again based on a suitable stability condition.

Finally, in *Chapter 6*, an adaptive timestep control will be devised in the improved contact–stabilized Newmark method (ContacX). On the basis of a theoretical and numerical investigation of an asymptotic error expansion of the Newmark scheme, established extrapolation techniques will be transferred to the algorithm in order to construct a comparative scheme of higher-order accuracy. This allows the suggestion of a problem-adapted error estimator and timestep selection which also cover the presence of contact. Moreover, the actually achieved global discretization error of the adaptive timestep control will be discussed. In *Chapter 7*, an illustrative numerical example will be given followed by a prototype of a dynamical simulation of a human knee joint.