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A computational framework for simultaneous estimation of muscle and joint contact forces and body motion using optimization and surrogate modeling

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ABSTRACT

Concurrent estimation of muscle activations, joint contact forces, and joint kinematics by means of gradient-based optimization of musculoskeletal models is hindered by computationally expensive and non-smooth joint contact and muscle wrapping algorithms. We present a framework that simultaneously speeds up computation and removes sources of non-smoothness from muscle force optimizations using a combination of parallelization and surrogate modeling, with special emphasis on a novel method for modeling joint contact as a surrogate model of a static analysis. The approach allows one to efficiently introduce elastic joint contact models within static and dynamic optimizations of human motion. We demonstrate the approach by performing two optimizations, one static and one dynamic, using a pelvis-leg musculoskeletal model undergoing a gait cycle. We observed convergence on the order of seconds for a static optimization time frame and on the order of minutes for an entire dynamic optimization. The presented framework may facilitate model-based efforts to predict how planned surgical or rehabilitation interventions will affect post-treatment joint and muscle function.

1. Introduction

Modeling and simulation of muscle and joint contact forces has the potential to improve patient care for movement-related disorders. Reliable concurrent estimation of these forces along with joint kinematics could be used to predict joint replacement performance, surgical outcomes, and rehabilitation strategies for a variety of musculoskeletal disorders. Most studies that predict muscle and joint contact forces model biological joints as constraint-based engineering joints. In those studies, muscle and joint contact forces are calculated by following a two-step process: (1) Muscle forces are computed using a multibody dynamic skeletal model and optimization, and then (2) Associated joint contact forces are calculated from knowledge of the muscle forces and joint reaction forces from inverse dynamics [1–4]. The downsides of this two-step approach are that it can produce erroneous muscle force predictions [5] and cannot predict secondary kinematics (e.g., knee anterior-posterior translation) or ligament forces for the joints being modeled.

For this reason, researchers have sought to develop more complex modeling methods that allow concurrent estimation of muscle and joint contact forces. Such methods replace constraint-based engineering joints with deformable joint surfaces whose interactions are controlled primarily by muscle and ligament forces. Lin et al. (2010) predicted muscle and knee contact forces simultaneously using a two-level optimization method where the outer level guessed the muscle force distribution and the inner-level found the corresponding static configuration of the joint using surrogate contact models [6]. These models approximated the input-output characteristics of elastic foundation contact models. Thelen et al. (2014) and Smith et al. (2016) used a modified version of computed muscle control (CMC), where a controller tracked desired accelerations while joint translational accelerations were assumed to be zero and an elastic foundation was used to model contact [7,8]. Marra et al. (2015) and Andersen et al. (2011, 2017) used force-dependent kinematics (FDK), where secondary joint coordinates were added as design variables within a static optimization [9–11]. With this approach, the velocities and accelerations of the secondary coordinates were assumed to be zero and an elastic foundation was used to model contact. In one recent study a surrogate contact model was used to speed up FDK computation [12]. Guess et al. (2014)

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avoided optimization and instead used feedback control with deformable contact models for the foot and joint of interest [13]. Moissenet et al. (2014) performed concurrent computation of muscle and contact forces within an optimization by using simplified joint models and Lagrange multipliers [14].

Unfortunately, developing optimization-based predictions of motion where muscle and joint contact forces are solved concurrently remains a difficult and computationally slow task. The primary reasons are the difficulties encountered when applying gradient-based optimization to musculoskeletal models with computationally costly and non-smooth (discontinuous or non-differentiable) contact models as well as non-smooth musculoskeletal geometry models (e.g., muscle-tendon lengths and moment arms). Contact models are computationally costly because they involve computing distances between complex three-dimensional surfaces and are non-smooth when various regions of the contacting surfaces come in to and out of contact. Moreover, contact forces and moments are sensitive to small pose variations that affect normal contact force, resulting in badly scaled gradients when pose parameters defining joint position and orientation are used as design variables [15]. Non-smoothness in muscle-tendon lengths and muscle moment arms can arise when muscles are modeled geometrically using sequences of line segments whose paths are determined by either wrapping objects or via points added or removed as a function of spanned joint angles [16–18]. Non-smoothness can be introduced when a line segment enters contact with a wrapping object, passes through a wrapping surface, snaps to the other side of a wrapping surface, or is rerouted by turning on or off a via point.

In this study, we propose a novel framework for performing concurrent muscle, joint contact, and joint kinematic simulations via optimization. We remove the non-smoothness problem while increasing computational efficiency by: (1) Generating surrogate models of deformable joint contact from finite element models and efficiently implementing them within optimizations using a novel approach, (2) Generating surrogate models of musculoskeletal geometry and using a custom Hill-type muscle-tendon model with rigid tendon, and (3) Parallelizing multibody dynamic model evaluations. The method results in the computationally efficient computation of non-linear constraints that are incorporated into static and dynamic optimizations of muscle and contact forces. In addition to describing the overall approach with special focus on surrogate contact modeling, we provide two illustrative examples to demonstrate implementation of the approach to knee contact and leg muscle force prediction. In the first example, we use a static optimization approach based on the existing FDK framework which we will call modified FDK (mod-FDK). In the second example, we formulate the same problem as a dynamic optimization and solve it using direct collocation.

2. Methods

2.1. Overview

The goal of our framework (Fig. 1) is to remove non-smoothness and computational expense from optimizations that predict muscle forces, joint contact forces, and joint motions simultaneously. We achieve this goal using a combination of surrogate modeling and parallelization. Surrogate modeling generates smooth and computationally inexpensive approximations of more computationally expensive models, while parallelization splits part of the computational load among multiple processors.

2.1.1. Key concepts

Before continuing with the methods, we first introduce several key concepts. The first concept is that of primary and secondary generalized coordinates. Secondary generalized coordinates are assumed to maintain a quasi-static equilibrium between muscle, ligament, and contact forces, disregarding the effect of inertial forces. The time derivatives of the secondary generalized coordinates are always assumed to be zero in our approach. Primary generalized coordinates are assumed to be affected by inertial forces, and thus their time derivatives are not assumed to be zero.

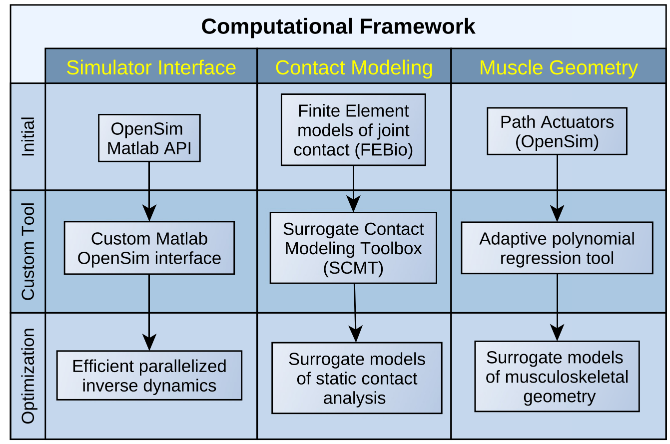

Fig. 1. Summary of computational framework for speeding up and removing non-smoothness from musculoskeletal optimization problems with joint contact. In the initial stage, joint contact is modelled using finite elements, muscle-tendon geometry using path actuators, and the simulator interface is the OpenSim API for Matlab. Three custom tools were developed which allowed us to obtain surrogate models of joint contact and musculoskeletal geometry, as well as an efficient simulation interface for deployment in the optimization stage.

Another important concept is that of static and dynamic optimization. A static optimization performs a minimization at a specified time point, while a dynamic optimization performs a minimization over some period of time. Dynamic optimization may also be known as trajectory optimization or optimal control. While a static optimization minimizes a cost function and is subjected to equality and/or inequality constraints, a dynamic optimizations minimizes a cost functional and is subjected to path constraints and possibly end-point constraints, though other types of constraints can be incorporated as well.

For contact modeling purposes, we also define the concept of a fixed body and a moving body. Since contact forces depend on the relative orientation of one body with respect to another, we define the fixed body as the contacting body that is conceptually fixed while the moving body is thought of as being translated and rotated by six pose parameters (3 translations and 3 rotations) relative to the fixed body.

A final important concept related to contact modeling is that of sensitive directions. A sensitive direction is defined as a degree of freedom (DOF), either translational or rotational, which when perturbed causes relatively large changes in the contact loads (forces and moments resulting from contact) associated with that DOF. The concept of sensitive directions is intimately related to surrogate contact model creation and optimization formulation.

2.1.2. About this framework

In inverse dynamics-based muscle force optimizations, the goal is to find the muscle activations (design variables) that minimize some assumed measure (e.g., fatigue or energy) while the joint forces and moments calculated via inverse dynamics are constrained to be balanced by a combination of muscle, ligament, and contact forces. The focus of our framework is on how to efficiently compute smooth non-linear constraints, representing the balancing of the net joint forces and moments. In the first part of the methods, we explain the general approach required to compute these