Rapid Predictive Simulations to Study the Interaction Between Motor Control and Musculoskeletal Dynamics in Healthy and Pathological Human Movement

Friedl De Groote and Antoine Falisse

Abstract We recently proposed a framework for rapid predictive simulations of human movement and demonstrated its potential to dissociate the contributions of neural and musculoskeletal impairments to gait deficits in cerebral palsy. Here, we give an overview of the framework and its applications, and demonstrate how using a more complex foot model was important to improve the correspondence between simulated and measured knee and ankle mechanics in a healthy individual.

1 Introduction

Scientists have long tried to decipher the principles underlying bipedal locomotion with the aim of improving human gait performance and treatment of neuromusculoskeletal disorders. A powerful approach to this problem is the use of physicsbased predictive simulations that generate de novo movements based on a mathematical description of the neuro-musculoskeletal system without relying on experimental data. However, the high computational time of predictive simulations has limited model complexity. Although simulations based on models with limited complexity have greatly contributed to our understanding of the mechanics and energetics of human gait, they provide limited support for personalized clinical decision-making. For example, an orthopaedic surgeon planning a single event multi-level surgery in a patient with cerebral palsy cannot predict the effect of the surgery on the walking pattern of the patient using a 2D model since such surgeries typically include 3D corrections of bony geometries.

We recently developed a computationally efficient optimal control framework to predict human gaits based on complex 3D musculoskeletal models [\[1\]](#page-4-0). Human gaits are predicted by optimizing a performance criterion that describes the high-level goal of the motor task without relying on experimental motion data. The framework's computational efficiency results from combining direct collocation, implicit

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F. De Groote (\boxtimes) \cdot A. Falisse

Department of Movement Sciences, KU Leuven, Leuven, Belgium e-mail: friedl.degroote@kuleuven.be

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differential equations, and algorithmic differentiation. Our framework is more than 20 times faster than existing simulations with similarly complex models.

The low computation time allowed us to explore the effect of the performance criterion on the predicted kinematics. We found a human like walking gait when minimizing a weighted sum of metabolic energy rate, muscle activity, joint accelerations, and passive joint torques—all terms squared. The same criterion also predicted the walk-to-run transition and clinical gait deficiencies caused by muscle weakness and prosthesis use, suggesting that diverse healthy and pathological gaits can emerge from the same control strategy.

In a follow-up study, we performed a case study to demonstrate the potential of our simulation framework to dissociate the contributions of motor control and musculoskeletal deficits to gait impairments in cerebral palsy [\[2\]](#page-4-1). We modeled altered musculoskeletal geometry based on MRI images, altered muscle-tendon properties by personalizing Hill-type muscle-tendon parameters based on data collected during functional movements, simpler neuromuscular control by reducing the number of independent muscle synergies, and spasticity through delayed muscle activity feedback from muscle force and force rate. Our simulations revealed that, in the presence of aberrant musculoskeletal geometries, altered muscle-tendon properties rather than reduced neuromuscular control complexity and spasticity were the primary cause of the crouch gait pattern observed for this child. Hence, our simulations suggested that muscle-tendon properties should be the primary intervention target for this child. Indeed, the gait pattern of the child was more upright following muscle-tendon property and bone deformity corrections.

Although we have demonstrated the ability of our simulations to reproduce key features of healthy and pathological human locomotion, our simulated walking patterns deviated from walking patterns observed in healthy individuals in two ways. First, we failed to predict knee flexion during mid stance, resulting in lower knee extension torques and vasti activity than experimentally observed. Second, our simulations underestimated ankle plantarflexion at push-off although the ankle torque was in good agreement with experimental data.

Here, we demonstrate that a more complex foot model including toes and a metatarsophalangeal joint was important to obtain physiologically plausible knee and ankle mechanics during stance.

2 Material and Methods

We performed simulations using two musculoskeletal models that only differed in the number of degrees of freedom used to represent the foot. The first model was an OpenSim model with 29 degrees of freedom, 92 Hill-type muscles actuating the lower limbs and trunk, and eight torque actuators at the arms [\[3,](#page-4-2) [4\]](#page-4-3). The second model was derived from the first model by adding an additional degree of freedom to the foot. The metatarsophalangeal joint had stiffness and damping properties inspired by experimental measures and was torque-actuated. We used Hunt-Crossley models to describe contact with the ground.

We formulated predictive simulations of gait as optimal control problems. We identified muscle excitations and gait cycle duration that minimized the cost function described above subject to constraints describing muscle and skeleton dynamics, imposing left–right symmetry and prescribing an average gait speed of 1.33 m/s. The resulting optimal control problems are typically challenging to solve because of the stiffness of the equations describing muscle and skeleton dynamics. Compared to other methods such as direct shooting, direct collocation reduces the sensitivity of the cost function to the optimization variables by reducing the time horizon of the integration. Applying direct collocation results in large sparse nonlinear programming problems (NLP). We improved the numerical conditioning of the NLP by using an implicit rather than explicit formulation of the muscle and skeleton dynamics. Additionally, we reduced computational time by applying algorithmic differentiation, rather than finite differences, to compute the derivatives required by the NLP solver.

Simulated kinematics, kinetics and muscle activities were evaluated against experimental data collected in one healthy adult. The subject walked overground at a selfselected speed of 1.33 \pm 0.06 m/s. The musculoskeletal model was scaled to the subject's anthropometry based on marker information from a standing calibration trial. Joint kinematics were calculated based on marker coordinates. Joint kinetics were calculated based on joint kinematics and ground reaction forces.

3 Results

The correspondence between measured and simulated kinematics, kinetics and muscle activations was markedly better when including the metatarsophalangeal joint in the model (Fig. [1\)](#page-3-0). Hip kinematics and kinetics were similar for both models. Modeling the toes was important to predict knee flexion, knee extension torque and vasti activity during stance. Modeling the toes increased ankle plantarflexion during push-off although initiation of the plantarflexion movement occurred sooner than experimentally observed.

4 Discussion

It has been suggested that a walking movement with knee flexion during mid-stance requiring a knee extension torque and thus activity of the vasti muscles is energetically less efficient but improves stability against internal and external perturbations [\[5\]](#page-4-4). Here, we demonstrate that knee flexion during mid-stance is optimal even when not accounting for robustness against perturbations. The main terms in our cost function were metabolic rate and muscle activity, which are both related to gait efficiency.

Fig. 1 Simulated and experimental gait kinematics, kinetics and muscle activities as a function of the gait cycle (heel contact to heel contact). Experimental data are shown as mean ± 2 standard deviations

Hence, if knee flexion is indeed needed for stability, stability and efficiency might not be conflicting requirements. We are currently extending our optimal control framework to a robust optimal control framework to study how robustness against perturbations shapes movement.

5 Conclusion

We expect that the ability to accurately and efficiently predict gait patterns based on complex musculoskeletal models will enable optimal design of treatments aiming to restore gait function in the future.

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