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DIRECT COLLOCATION, IMPLICIT DIFFERENTIAL EQUATIONS, ALGORITHMIC DIFFERENTIATION: A COCKTAIL FOR RAPID PREDICTIVE SIMULATIONS OF MOVEMENT BASED ON COMPLEX MUSCULOSKELETAL MODELS

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INTRODUCTION

Scientists have long tried to decipher the principles underlying bipedal locomotion with the aim of improving human gait performance and treatment of neuro-musculoskeletal disorders. An approach to this problem is the use of forward dynamic simulations. Such simulations can be used for tracking measured movements or for predicting *de novo* movements by optimizing a movement-related performance criterion (e.g., metabolic cost) without relying on measured data. Predictive simulations hold a great potential but are computationally expensive when based on complex musculoskeletal models [1-2]. Therefore, the field has not explored their ability to predict the range of gaits encountered under different environments, pathologies, and augmentations.

We have developed a computationally efficient optimal control framework to generate forward dynamic simulations based on complex musculoskeletal models. The framework's computational efficiency results from combining direct collocation, implicit differential equations, and algorithmic differentiation (AD). Here, we first demonstrate how using AD instead of more common finite differences (FD) drastically improves computational (CPU) time of forward dynamic simulations. Then, we rely on our framework to generate three-dimensional (3D) muscle-driven predictive simulations of gait. Our 3D predictive simulations converge on average in 36 minutes of CPU time on a single core of a standard laptop computer, which is more than 20 times faster than existing simulations with similarly complex models [1-2]. This efficiency allowed us to test the ability to predict the mechanics and energetics of a range of human gaits based on complex models. This is a prerequisite to rely on such models for optimal treatment design.

METHODS

We formulated forward dynamic simulations as optimal control problems. We computed muscle excitations by minimizing a cost function subject to constraints describing musculoskeletal dynamics. We first performed predictive and tracking simulations of walking with 2D and 3D musculoskeletal models, respectively, while comparing AD and FD. For the 2D predictive simulations, we minimized the sum of muscle activations squared while imposing left-right symmetry and average gait speed. For the 3D tracking simulations, we minimized the difference between measured and model variables (joint kinematics, kinetics, ground reaction forces and moments) as well as muscle effort. We then performed 3D predictive simulations of gait in which we minimized a weighted sum of metabolic energy rate, muscle activity, and joint accelerations while imposing left-right symmetry and average gait speed. In particular, we tested whether our framework was generalizable by predicting gait at different speeds, with muscle strength deficits, and with a lower leg prosthesis. We compared our 3D simulation results from these diverse conditions to those from experiments.

The resulting nonlinear optimal control problems are challenging to solve because of the stiffness of the equations describing the musculoskeletal dynamics. Due to these stiff equations, a small change in muscle excitations can have a large impact on the simulated movement pattern and the cost function because of, for example, the high sensitivity of the ground reaction forces to the kinematics. To overcome this challenge, we used an optimal control method called direct collocation [3]. Compared to others 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) that can be solved efficiently by readily available NLP solvers. We further improved the numerical conditioning of the NLP by formulating the musculoskeletal dynamics with implicit rather than explicit differential equations [3]. To this aim, we introduced additional controls that are the time derivative of the states. The implicit dynamic equations were then imposed as path constraints. Additionally, we reduced CPU time by using AD rather than FD to compute derivatives required by the NLP solver [4]. AD provides exact derivatives and permits the evaluation of a Jacobian-transposed vector product through its reverse mode. Depending on the problem dimensions and sparsity, the reverse mode can decrease the number of function evaluations required to evaluate the matrices required by the NLP solver. We created a custom version of OpenSim [5] to enable AD of the multi-body dynamics. We formulated all problems in MATLAB with CasADi [4], using a third order Radau quadrature collocation scheme and the solver IPOPT.

RESULTS AND DISCUSSION

AD was between 10 and 21 times faster than FD to solve 2D predictive and 3D tracking simulations (Table 1). Specifically, AD's reverse mode allowed drastically decreasing the CPU time spent in evaluating the objective function gradient, which led to faster convergence.

Table 1. Computational time required to solve forward dynamic simulations (mean ± standard deviation when solving same problem from different initial guesses).

	AD	FD
2D predictive simulations	36 ± 17 (s)	374 ± 210 (s)
3D tracking simulations	19 ± 7 (min)	334 ± 25 (min)

Our 3D predictive simulations produced a continuum of walking and running gaits when we varied the prescribed gait speed from 0.73 to 2.73 ms^{-1} using the same control strategy (i.e., cost function). Further, the metabolic cost of transport (COT) and stride frequency changed as a function of speed in agreement with reported data (Fig 1A) [6-7]. A transition from walking to running occurred at 2.23 ms^{-1}. Our simulations demonstrate that walking and running can emerge from the same underlying control strategy, providing further support for observations based on experiments and conceptual models that did not account for the large redundancy in the musculoskeletal system.

Altering musculoskeletal properties led to gaits that exhibited clinical gait deficiencies. We simulated gait while either weakening all hip muscles or the ankle plantarflexors by decreasing the maximal isometric muscle forces. Reduced hip muscle strength led to greater hip circumduction to reduce hip torques (Fig 1B, left); a strategy, known as compensated Trendelenburg gait, which may be observed in patients with neural injuries or myopathies affecting hip muscles [8]. Reduced ankle plantarflexor strength resulted in crouch and calcaneal gaits that reduced ankle torques (Fig 1B, right). Such gaits may be observed in children with spastic diplegia who have a weak triceps surae, due to an Achilles tendon lengthening surgery [9].

Our simulations produced ankle torques and COT that are typical of amputees with a transtibial passive prosthesis (Fig 1C). Ankle torques of the affected leg were larger during early- and mid-stance than the torques of the unaffected leg [10]. The COT was similar to the COT of a healthy subject, as expected for physically fit amputees.

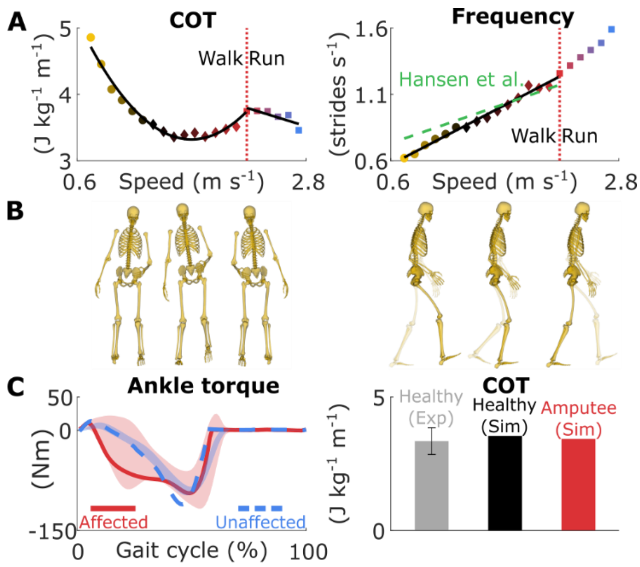

Fig 1: Effect of (A) varying gait speed, (B) weakening all hip muscles (left) or the ankle plantaflexors (right), and (C) wearing a transtibial passive prosthesis (Exp: experiment [2]; Sim: simulation).

CONCLUSIONS

The computational efficiency of our framework, in part due to AD, allowed us to demonstrate the ability to predict the mechanics and energetics of a range of gaits with complex models. We expect these predictions to enable optimal design of treatments aiming to restore gait function.

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