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Femoral strain during walking predicted with muscle forces from static and dynamic optimization

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ABSTRACT

Mechanical strain plays an important role in skeletal health, and the ability to accurately and non-invasively quantify bone strain *in vivo* may be used to develop preventive measures that improve bone quality and decrease fracture risk. A non-invasive estimation of bone strain requires combined musculoskeletal – finite element modeling, for which the applied muscle forces are usually obtained from static optimization (SO) methods. In this study, we compared finite element predicted femoral strains in walking using muscle forces obtained from SO to those obtained from forward dynamics (FD) simulation. The general trends in strain distributions were similar between FD and SO derived conditions and both agreed well with previously reported *in vivo* strain gage measurements. On the other hand, differences in peak maximum (ε_{max}) and minimum (ε_{min}) principal strain magnitudes were as high as 32% between FD ($\varepsilon_{max}/\varepsilon_{min}=945/-1271$ με) and SO ($\varepsilon_{max}/\varepsilon_{min}=752/-859$ με). These large differences in strain magnitudes were observed during the first half of stance, where SO predicted lower gluteal muscle forces and virtually no co-contraction of the hip adductors compared to FD. The importance of these results will likely depend on the purpose/application of the modeling procedure. If the goal is to obtain a generalized strain distribution for adaptive bone remodeling algorithms, then traditional SO is likely sufficient. In cases were strain magnitudes are critical, as is the case with fracture risk assessment, bone strain estimation may benefit by including muscle activation and contractile dynamics in SO, or by using FD when practical.

1. Introduction

Bone is a dynamic tissue that exhibits a strong structure-function relationship with its mechanical loading environment. Indeed, physically active individuals tend to accrue more bone mass during growth and development, and better maintain this bone mass throughout adulthood, than their more sedentary counterparts (Parfitt, 1994). Additionally, the loss of ambulation and habitual muscle loading associated with bed rest or paralysis leads to a rapid and profound loss of bone mineral (Edwards et al., 2013a). In the complete absence of mechanical loading bone reverts to its genetic template, normal in shape and size but lacking distinct characteristics in trabecular microarchitecture, the amount of ossification, and thickness and curvature of the cortical diaphysis (Chalmers and Ray, 1962).

The process by which bone senses and responds to mechanical loading is known as functional adaptation, and the mechanical signal that drives this adaptive process is bone strain (Lanyon and Skerry, 2001), or some consequence thereof (i.e., strain energy density, fluid flow, microdamage). An accurate estimation of bone strain during activities of daily living such as walking is therefore integral to understanding the relationship between mechanical loading and skeletal health. In the physiological environment, bone strain is the end result of highly complex loading scenarios (i.e., combined axial, bending, shear, and torsional loading) caused by both gravitational and muscular forces. The resulting bone strain can be quantified *in vivo* using strain gages applied directly to the periosteal surface (Burr et al., 1996); however, the application of strain gages is highly invasive and measurements are limited to only a few, superficial locations. Owing to these limitations, researchers have turned to combined musculoskeletal – finite element modeling techniques for a more non-invasive estimation

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of bone strain (Anderson and Madigan, 2013; Speirs et al., 2007; Vahdati et al., 2014; Viceconti et al., 2012; Wagner et al., 2010).

The concurrent solving of musculoskeletal – finite element models is highly computationally intensive. Methods for estimating muscle forces from musculoskeletal models can require hundreds, thousands, or even millions of iterations within numerical optimization routines (Erdemir et al., 2007), and spending hours or even minutes within each iteration solving a finite element model would incur an impractical amount of computational time. As such, it is most common to use a post-processing technique whereby muscle forces derived from a higher-level rigid multibody simulation are used as boundary conditions for a lower-level elastic model to quantify bone strain (Anderson and Madigan, 2013; Speirs et al., 2007; Vahdati et al., 2014; Viceconti et al., 2012; Wagner et al., 2010). Inherent to a post-processing approach is the assumption that the underlying elastic deformation has no influence on the dynamics of the rigid multibody system. For the calculation of bone strain, this assumption is logical given that bone deformation (Burr et al., 1996) is orders of magnitude lower than that of the musculotendonous units (Fukunaga et al., 2001) and would theoretically have a negligible influence on whole-body motion.

The redundancy of the musculoskeletal system allows for an infinite number of muscle force combinations capable of producing the observed joint motions during physical activity (Crowninshield and Brand, 1981). This so-called “force-distribution problem” is typically overcome using numerical optimization procedures (Erdemir et al., 2007). For researchers using combined musculoskeletal – finite element modeling techniques, muscle forces are most frequently predicted using inverse dynamics-based static optimization (Anderson and Madigan, 2013; Speirs et al., 2007; Vahdati et al., 2014; Wagner et al., 2010). Static optimization is much less computationally intensive than dynamic optimization, which uses forward dynamics simulation to find optimal motions and controls for a given performance objective, such as tracking an experimental dataset and/or minimizing the metabolic energy expended. Although muscle forces from static optimization and forward dynamics have previously been deemed similar for walking (Anderson and Pandy, 2001b), static optimization has been criticized for lacking explicit time-dependent aspects of muscle force production, and for predicting minimal levels of antagonistic muscle co-contraction (Brand et al., 1994; Collins, 1995), which could potentially have a large influence on overall bone deformation and corresponding strain predictions.

The purpose of this study was to quantitatively evaluate finite element predicted periosteal strains at the femur during walking using muscle forces estimated from static and dynamic optimization. To this end, a previously described forward dynamics (FD) simulation of walking was performed using a 3D musculoskeletal model (Fig. 1), and intersegmental joint moments from FD were subsequently used in an inverse-dynamics-based static optimization (SO) routine. The muscle forces obtained from FD and SO served as post-possessing inputs to a finite element (FE) model of a femur based on clinical computed tomography (CT) data, and the resulting periosteal strains were compared between FD and SO derived conditions.

2. Methods

2.1. Musculoskeletal modeling

A 3D musculoskeletal model (Fig. 1c) parameterized to represent a young adult female (i.e., 20–35 years) with standing height of 1.65 m and body mass of 61.0 kg was used to simulate walking at 1.25 m/s. The model was conceptually similar to other models used to perform FD gait simulations (Allen and Neptune, 2012; Anderson and Pandy, 2001a) and has been previously described in detail (Miller et al., 2015). Briefly, the model consisted of 10 rigid segments (pelvis, trunk, thighs, shanks, feet, toes) connected at nine joints actuated by 78 Hill-based muscle models (Fig. 1b), including 20 muscles per leg that crossed the hip and/or physically connected to the femur. Contact between the feet and the ground was modeled by an array of viscoelastic/Coulomb friction elements on the plantar surfaces of the feet and toe segments. Initial muscle parameters were referenced from a cadaver-based lower limb model (Arnold et al., 2010), which were then adjusted so that joint strength characteristics were similar to average dynamometry data for young adult females (Anderson et al., 2007).

2.1.1. Forward dynamics simulation

A simulation of one stride of periodic, bilaterally symmetric walking was performed using a dynamic optimization routine described in our previous work (Miller et al., 2012, 2015) and by others (Allen and Neptune, 2012; Umberger, 2010). Briefly, the muscle excitations were parameterized as bimodal signals with two magnitude and four timing parameters per muscle (Fig. 1a). The excitation parameters were optimized to track human experimental gait data (Miller et al., 2014). Specific gait variables included in the tracking cost function were average time series for the pelvis (3D), lumbar (3D), hip (3D), knee (1D), and ankle (1D) angles, the ground reaction force (3D), and the knee adduction moment. To discourage solutions that tracked these data with excessive energy expenditure, the metabolic energy per unit distance traveled was also calculated (Umberger et al., 2003) and added to the cost function (see Electronic Supplementary Material for details). A parallel simulated annealing algorithm (SPAN; Higginson et al., 2005) was used to systematically adjust muscle excitation parameters so that the cost function was minimized (Fig. 1d). Muscle excitation timings for larger muscles were constrained to be similar to normative human electromyogram timing (Sutherland, 2001).

2.1.2. Inverse dynamics based static optimization

An inverse dynamics analysis was performed using data obtained from FD simulation to calculate the intersegmental joint forces and moments. The joint moments and muscle moment arms were used as inputs to a SO problem similar to our previous work (Edwards et al., 2010; Miller et al., 2014), which was solved using the interior-point algorithm in the Matlab Optimization Toolbox. At each time step of the simulated gait cycle, the muscle forces were determined such that (i) all joint moments from the inverse dynamics analysis were reproduced (equality constraint) and (ii) the sum of the squared muscle stresses was minimized (Glitsch and Baumann, 1997). This approach, which is conceptually similar to that of Anderson and Pandy (2001b), was chosen to eliminate differences between muscle forces from FD and SO associated with errors in the collection and processing of experimental data, and the estimation of segment anthropometry. All muscles were modeled as ideal force generators with no contractile or elastic properties because previous studies have suggested adjusting solution boundaries by activation dynamics has a negligible influence on muscle force predictions in walking (Anderson and Pandy, 2001b).

2.2. Finite element modeling

A FE model of a full femur was obtained from the VAKHUM database (http://www.ulb.ac.be/project/vakhum/). The native geometry and material properties of the model were based on clinical CT data from a female cadaver (age: 99 years, height: 155 cm, mass: 55 kg). The CT scan had acquisition setting of 120 kVp and 200 mAs, and images were reconstructed with a slice thickness of 2.7 mm and an in-plane pixel resolution of 0.840 mm. The FE model was comprised of 104,945 linear hexahedral elements with 115,835 degrees of freedom, corresponding to a nominal element edge length of 2.0 mm. Increasing element edge length from 2.0 to 3.0 mm changed femoral displacements, principal stresses, and principal strains by less than 3%, indicating adequate convergence at this refinement.

The FE model was first scaled longitudinally to the femoral body of the musculoskeletal model, and then scaled radially assuming bone mass scales to body mass, or length $\cdot$ diameter$^2 \propto$ body mass (McMahon, 1973), as further justified by the observed correlations between whole-body bone mineral content and body mass (Weiler et al., 2000). Elements were assigned to one of 283 linear-elastic material properties based on relationships between Hounsfield units and apparent density after the integral volumetric bone mineral density of the entire femur was increased by 26% to match that of a young adult female (Keaveny et al., 2010). The density–elasticity relationship was based on uniaxial mechanical testing data of femoral neck trabecular bone (Morgan et al., 2003):

$$E = 6850\rho_{app}{}^{1.49}$$

where E is the elastic modulus in MPa, and ρ_{app} is the apparent density in g/cm^3; all materials were assigned a Poisson's ratio of 0.3. These material property assignments have previously illustrated excellent agreement (r^2=0.91, RMSE < 10%) between experimentally measured and FE-predicted principal strains for cadaveric proximal femora loaded in a stance configuration (Schileo et al., 2007).

An affine iterative-closest-point registration procedure available from Matlab Central File Exchange (http://www.mathworks.com/matlabcentral/fileexchange/24301-finite-iterative-closest-point) was used to align the FE and musculoskeletal model femur into a common local coordinate system. Femoral muscle insertion locations from the musculoskeletal model were then mapped to surface nodes of the FE model. Forces for each of the gluteal muscles (i.e., maximus, medius, and