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What is This?
Prediction of in vivo joint mechanics of an artificial knee implant using rigid multi-body dynamics with elastic contacts

Zhenxian Chen¹, Xuan Zhang¹, Marzieh M Ardestani¹, Ling Wang¹, Yaxiong Liu¹, Qin Lian¹, Jiankang He¹, Dichen Li¹ and Zhongmin Jin¹,²

Abstract
Lower extremity musculoskeletal computational models play an important role in predicting joint forces and muscle activation simultaneously and are valuable for investigating functional outcomes of the implants. However, current computational musculoskeletal models of total knee replacement rarely consider the bearing surface geometry of the implant. Therefore, these models lack detailed information about the contact loading and joint motion which are important factors for evaluating clinical performances. This study extended a rigid multi-body dynamics simulation of a lower extremity musculoskeletal model to incorporate an artificial knee joint, based upon a novel force-dependent kinematics method, and to characterize the in vivo joint contact mechanics during gait. The developed musculoskeletal total knee replacement model integrated the rigid skeleton multi-body dynamics and the flexible contact mechanics of the tibiofemoral and patellofemoral joints. The predicted contact forces and muscle activations are compared against those in vivo measurements obtained from a single patient with good agreements for the medial contact force (root-mean-square error = 215 N, ρ = 0.96) and lateral contact force (root-mean-square error = 179 N, ρ = 0.75). Moreover, the developed model also predicted the motion of the tibiofemoral joint in all degrees of freedom. This new model provides an important step toward the development of a realistic dynamic musculoskeletal total knee replacement model to predict in vivo knee joint motion and loading simultaneously. This could offer a better opportunity to establish a robust virtual modeling platform for future pre-clinical assessment of knee prosthesis designs, surgical procedures and post-operation rehabilitation.

Keywords
Musculoskeletal model, multi-body dynamics, force-dependent kinematics, total knee replacement, muscle activation, contact force

Introduction
The total knee replacement (TKR) is an effective way to replace the damaged knee joints and help the patient restore daily activities. However, wear and aseptic loosening, resulted from wear particles, still restrict the clinical lifetime of TKRs. Functional outcomes of current TKR implants are highly affected by the contact mechanics, joint kinematics, and wear of joint components.¹ Joint motion,² dynamic loading,³ and the stability from muscles and ligaments may contribute to the knee implant failures. Thus, knowledge of in vivo muscle interaction, joint motion, and joint contact forces during functional activities is essential to understand the failure mechanisms and improve the performance of the implanted knee joints.

Instrumented knee implants with force-sensing transducers provide the feasibility of real-time quantitative

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evaluation of the joint contact forces during a gait cycle to investigate in vivo knee joint dynamics. However, using these instruments might not be always straightforward, especially to study the effect of different surgical malalignments or implant designs on dynamic loading and motion. Although dynamic finite element knee models, such as the one by Fitzpatrick et al., are an attractive alternative for predicting knee contact forces and motion, a host of musculoskeletal (MSK) multi-body dynamics (MBD) models with varying complexity and authenticity have been developed.

More recently, many MBD software packages have been introduced to model the MSK system. The lower extremity MSK models, once experimentally validated, have been used widely to simulate and estimate both joint loading and muscular actions. The majority of these dynamics models developed are based on the assumption of rigid body, with no deformation involved, to determine joint loading. Finite element models are subsequently employed to predict the contact stresses with the detailed joint components using the load and motion profiles determined from the MBD model. Thus, an ideal computational model should combine an MBD MSK model to predict muscle forces with a deformable contact model considering the implant surface geometry to predict contact mechanics simultaneously. However, such three-dimensional multi-body knee models published in the literature have revealed computational challenges. The majority of previous MSK models have assumed an idealized revolute knee joint so that to constrain the thigh and the shank as a convenience in inverse dynamics analysis. Additionally, the majority of the reported TKR models have neglected the influence of ligaments and muscles on contact forces and the elastic contact in joint mechanics analysis. A review of typical representative TKR MBD studies is summarized in Table 17–19 to highlight the differences of the lower extremity MSK models and reported output parameters (contact modeling and MBD modeling are also included for reference). There are few studies in which the articular geometry of the TKR model has been taken into account, and muscle activation and medial and lateral contact forces are predicted and reported simultaneously during gait simulation. Some models, such as the one reported by Williams et al., were developed to simulate a knee simulator machine–driven gait cycle where the focus was more on the predicted contact stresses in comparison to the measured wear surface of the retrieved implant component modeled in the gait simulation. Moreover, the relative motions of the knee joint components are governed by a complex interaction between the muscle actions, ligament forces and implant contact surface deformation and are rarely predicted in previous MSK modeling studies. Although these models possess a number of limitations, significant advances have been made. Especially, notable developments are the modular modeling approach based on the elastic foundation or a “bed of springs” theory that permits the incorporation of a deformable knee model into a MBD simulation environment. The method has been experimentally validated for predicting contact pressure distribution and widely used in TKR studies. The elastic foundation model employing non-linear polyethylene material properties was constructed to calculate the medial and lateral contact forces resulted from the measured kinematics. Stylianou et al. have recently incorporated the elastic foundation TKR model into a full MSK MBD environment under squatting. Meanwhile, a force-dependent kinematics (FDK) model has been introduced to allow the non-conforming knee and the articular geometries being simulated to replace the idealized revolute joint model for predicting the relative internal motions that are not predetermined in specified directions. FDK is based on an assumption of quasi-static force equilibrium between all the acting forces in the model in the directions of motion. This method can be potentially used to predict the joint reaction force and muscle forces as well as the joint motion simultaneously. In general, almost all of the studies including the elastic deformation of the contacting surfaces of TKRs have assumed simplified MSK models, while full MSK models have rarely considered TKR and bearing surface deformation in detail. It is possible to combine both approaches by coupling the rigid dynamics analysis and elastic contact analysis together for a more realistic and comprehensive prediction of the mechanical behavior of TKRs. In addition, patellar tracking and corresponding contact mechanics are equally important, as part of the knee system. However, a comprehensive study based on this coupled approach has not been carried out in the literature involving both femoral–tibial and femoral–patellar articulations in gait cycles.

In this study, a subject-specific MSK TKR model, considering lower extremity MSK MBD, contact mechanics of articular surfaces, and ligaments, was developed based on the elastic foundation theory and FDK. The medial and lateral tibiofemoral (TF) joint forces, patellofemoral (PF) joint force, internal TF joint motions, and muscle activations were predicted simultaneously in the developed knee model during a normal gait cycle.

Materials and methods

Experimental data

All related experimental data of an adult female subject implanted with an instrumented knee replacement (mass 78.4 kg, height 167 cm, left knee) used in this study were obtained from online resources (https://simtk.org/home/kneeloads, accessed on 27 February 2013). A second-generation instrumented knee design with a standard ultra-high-molecular-weight polyethylene (UHMWPE) insert and patellar button (NK-II CR Congruent; Zimmer) and a posterior cruciate-retaining cobalt-chromium-molybdenum (CoCrMo) femoral
<table>
<thead>
<tr>
<th>References</th>
<th>Knee contact modeling</th>
<th>MBD simulation</th>
<th>MSK models</th>
<th>Input (mainly mentioned)</th>
<th>Output (mainly reported)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fregly et al.(^7) and Zhao et al.(^8)</td>
<td>Elastic foundation theory (Pro/MECHANICA MOTION)</td>
<td>Forward dynamics</td>
<td>Only femoral component and tibial insert</td>
<td>Measured tibial force, AP translation, IE rotation, FE</td>
<td>Medial and lateral contact forces, contact pressure</td>
</tr>
<tr>
<td>Lin et al.(^9)</td>
<td>Surrogate contact modeling methods (AUTOLEY symbolic manipulation software + MATLAB)</td>
<td>Inverse dynamics</td>
<td>11 muscles and patellar ligament, femur, tibia, fibula, patella, TKR components</td>
<td>Overground gait data and additional isolated joint motion trials</td>
<td>Medial and lateral contact forces, patellar contact force, muscle forces</td>
</tr>
<tr>
<td>Gerus et al.(^10)</td>
<td>The point contact method without penetration (OpenSim)</td>
<td>Inverse dynamics</td>
<td>A whole lower extremity MSK model, TKR components</td>
<td>EMG activity from eight muscles, motion capture markers data, AP and IS translation</td>
<td>Medial and lateral contact forces, muscle forces, moment arms of selected major muscles AP translation and IE rotation</td>
</tr>
<tr>
<td>Lin et al., (^11) Liu et al., (^12) and Wang et al.(^13)</td>
<td>Solid to solid contact with Coulomb friction (MSC ADAMS)</td>
<td>Not mentioned</td>
<td>Ligament model and quadriceps, distal femur, proximal tibia, patella and fibula, TKR components</td>
<td>Ground reaction force, FE</td>
<td></td>
</tr>
<tr>
<td>Innocenti et al., (^14) Mihalko and Williams, (^15) Pianigiani et al., (^16) and Williams et al. (^17)</td>
<td>A damping and penetration algorithm with Coulomb friction (LifeMOD/KneeSIM, plug-in to the MSC ADAMS)</td>
<td>Forward dynamics</td>
<td>Ligament model, quadriceps and hamstrings, bones and TKR components (simulation of an existing knee kinematics rig)</td>
<td>Hip force, quadriceps, and hamstrings forces</td>
<td></td>
</tr>
<tr>
<td>Stylianou et al.(^18)</td>
<td>A damping and penetration algorithm with Coulomb friction (ADAMS + LifeMOD)</td>
<td>Forward dynamics</td>
<td>A whole lower extremity MSK model, TKR components; ligament model</td>
<td>Motion capture markers data</td>
<td>Tibial component forces and torques; muscle activation; joint kinematics; ground reaction forces; contact pressure</td>
</tr>
<tr>
<td>Andersen and Rasmussen (^19)</td>
<td>Elastic foundation theory + force-dependent kinematics (AnyBody)</td>
<td>Inverse dynamics</td>
<td>A whole lower extremity MSK model, TKR components; ligaments model</td>
<td>Motion capture markers data, ground reaction forces</td>
<td>Medial and lateral contact forces</td>
</tr>
</tbody>
</table>


The artificial bearing geometry of knee implants was considered in all the presented studies.
component (NK-II CR; Zimmer) were implanted using a standard anteromedial approach. The knee contact forces at the medial and lateral compartments were measured using force-sensing devices. In total, 15 electromyography (EMG) signals, marker trajectories, and analog force plate data associated with the normal gait pattern were used in this study. These measured muscles included biceps femoris long head, semimembranosus, vastus medialis, vastus lateralis, rectus femoris, medial gastrocnemius, lateral gastrocnemius, tensor fasciae latae, tibialis anterior, peroneus longus, soleus, adductor magnus, gluteus maximus, gluteus medius, and sartorius. For the purpose of evaluating the predicted muscle activation, EMG-to-activation model was adopted to represent the underlying muscle activation dynamics. Details of the transformation from EMG to muscle activation have been previously reported in the literature.

TKR computational model
The patient-specific lower extremity MSK model was developed in the commercial MSK simulation software AnyBody (version 6.0; AnyBody Technology, Aalborg, Denmark). To mitigate the challenges of the development of a full patient-specific model, the generic lower extremity MSK model was extracted from AnyBody Managed Model Repository (version 1.5.1) and modified for this study. The generic lower extremity MSK model is based on the Twente Lower Extremity Model (TLEM) anthropometric database. The hip is modeled as a spherical joint, and the knee, ankle, and subtalar joints are modeled as revolute joints. The MSK model is actuated by approximately 160 muscle units. The MSK model has been previously validated in the literature for predicting muscle forces and joint reaction forces in the human lower limb during locomotion.

In this study, the patient-specific bone and implant geometries (the femoral component, the tibial insert, and the patella button) were reverse-engineered from computed tomography (CT) scans released in the published database and imported into AnyBody to replace the existing left leg of the generic lower extremity MSK model (Figure 1). The other segments of the generic lower extremity MSK model were scaled on the basis of the subject’s weight, height, as well as the relative positions of the ankle, knee, and hip joints determined from the bone geometries. A Length–Mass–Fat scaling law, based on the segment distances between bony landmarks, was used in the scaling process. The fat percentage dependence on the body height and body mass was taken into account in the scaling law. Other scaling laws, including Length scaling law and Length–Mass scaling law, were also considered for parametric sensitivity analysis. Meanwhile, muscle attachment sites and geometries were scaled in accordance with a linear geometry scaling law. The marker coordinates relative to the segments were also estimated at the same time when the segments were scaled and
Table 2. Summary of the material constants$^{2,8}$ used in this study.

<table>
<thead>
<tr>
<th>Ligament</th>
<th>Ligament bundle</th>
<th>Stiffness parameter k (N)</th>
<th>$\dot{e}_v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCL</td>
<td>a</td>
<td>9000</td>
<td>-0.24</td>
</tr>
<tr>
<td></td>
<td>p</td>
<td>9000</td>
<td>-0.03</td>
</tr>
<tr>
<td>MCL</td>
<td>a</td>
<td>2750</td>
<td>0.04</td>
</tr>
<tr>
<td></td>
<td>i</td>
<td>2750</td>
<td>0.04</td>
</tr>
<tr>
<td></td>
<td>p</td>
<td>2750</td>
<td>0.03</td>
</tr>
<tr>
<td>LCL</td>
<td>a</td>
<td>2000</td>
<td>-0.25</td>
</tr>
<tr>
<td></td>
<td>s</td>
<td>2000</td>
<td>-0.05</td>
</tr>
<tr>
<td></td>
<td>p</td>
<td>2000</td>
<td>0.08</td>
</tr>
<tr>
<td>PMC</td>
<td>a</td>
<td>1000</td>
<td>-0.18</td>
</tr>
<tr>
<td></td>
<td>p</td>
<td>1000</td>
<td>-0.04</td>
</tr>
<tr>
<td>MPFL</td>
<td>s, i</td>
<td>2000</td>
<td>0.03</td>
</tr>
<tr>
<td>LPFL</td>
<td>s, i</td>
<td>2000</td>
<td>0.03</td>
</tr>
</tbody>
</table>

PCL: posterior cruciate ligament; MCL: medial collateral ligament; LCL: lateral collateral ligament; PMC: posterior-medial capsule; MPFL: medial PF ligament; LPFL: lateral PF ligament; PF: patello-femoral.

positioned. For more details on scaling of the lower extremity MSK modeling, one can refer to a previous study.$^{25}$

Six capsular soft tissue structures crossing the TF and PF joints available in AnyBody were adopted for the left leg of the modified lower extremity MSK model, including posterior cruciate ligament (PCL), medial collateral ligament (MCL), lateral collateral ligament (LCL), posterior-medial capsule (PMC), medial PF ligament (MPFL), and lateral PF ligament (LPFL). Anterior cruciate ligament (ACL) was removed by the surgery. These ligaments are modeled in AnyBody as non-linear spring elements with the following piecewise force–displacement relationship$^{28}$ according to their functional bundles based on actual ligament anatomy

$$f = \begin{cases} 0.25k\varepsilon^2/\varepsilon_l & 0 \leq \varepsilon \leq 2\varepsilon_l \\ k(\varepsilon - \varepsilon_l) & \varepsilon > 2\varepsilon_l \\ 0 & \varepsilon < 0 \end{cases}$$

(1)$$e = \frac{L - L_0}{L_0}; L_0 = \frac{L_\text{r}}{\dot{e}_v + 1}$$

(2)

where $f$ is the applied force, $k$ is the ligament stiffness parameter, $\varepsilon_l$ is a constant non-linear strain parameter of 0.03, $\varepsilon$ is the strain in the ligaments, $L$ is the ligament length, and $L_0$ is the zero-load length of the ligament (determined from the ligament’s initial length $L_\text{r}$ and the reference strain $\dot{e}_v$). The material parameters for these ligaments and capsules were taken from the literature and are shown in Table 2.$^{2,8}$

For the left knee of the modified lower extremity MSK model, the hinge joint definition was removed, and an anatomical left knee with the implant was created via the following FDK approach.$^{19}$ Due to the lack of the anatomical geometry of the patient’s right leg and the purpose for saving computational time, the hinge joint definition of the right knee was preserved. The equilibrium of the left knee was maintained from the balance between muscle, ligaments, and articular contact forces. Two deformable contact models were defined between the tibial insert and femoral component bearing surfaces and between the patellar button and the femoral component. The tibial insert was divided into medial and lateral compartments with separate contacts created for each. The contact force between the two objects represented with the contacting surfaces (in STereoLithography (STL) format) was calculated using a linear force-penetration volume law.$^{20}$ The contact pressure module PressureModule in Newton per meter cube is the key parameter in the default FDK computational framework of AnyBody. Due to the contact model implemented in AnyBody being very close to the elastic foundation theory,$^{20}$ the equations derived by Fregly et al.$^{20}$ according to the elastic foundation theory were used for the calculation of the PressureModule defined as below (equation (6)). For completeness, the governing equations, taken from Fregly et al.$^{20}$ are presented as follows

$$\frac{p}{d} = \frac{(1 - \nu)E(p)}{(1 + \nu)(1 - 2\nu)h}$$

(3)

where $p$ and $d$ are contact pressure and surface overclosure, respectively; and $E(p)$, $\nu$, and $h$ are Young’s modulus, Poisson’s ratio, and the local thickness of the UHMWPE tibial layer, respectively; and $d$ is the element’s spring deflection, defined as the interpenetration of the undeformed surfaces in the direction of the local surface normal. For a non-linear material, the elastic modulus was set as a function of the current level of contact pressure for each element. The following equation was taken from a non-linear power law material model$^{20}$

$$\varepsilon = \frac{1}{2} \varepsilon_o \frac{p}{p_o} + \frac{1}{2} \varepsilon_o \left(\frac{p}{p_o}\right)^n$$

(4)

where $\varepsilon$ is the strain, $p$ is the contact pressure, $\varepsilon_o = 0.0597$, $p_o = 18.4$ MPa, and $n = 3$ based on the experimental stress strain data for UHMWPE.$^{30}$ To take the derivative of $p$ over $\varepsilon$, and replace with $E(p) = dp/d\varepsilon$, equation (4) was rewritten as

$$E(p) = \frac{1}{\frac{1}{p_o} \left\{1 + n \left(\frac{p}{p_o}\right)^{n-1}\right\}}$$

(5)

Equation (5) was substituted into equation (3) to generate a single non-linear equation for $p$ and $d$ which was solved using a standard root-finding method. Further details for elastic foundation contact model can be found in the literature.$^{3,20}$

In this study, the UHMWPE was considered as a non-linear material, and its elastic modulus was at least two orders of magnitude lower than that of the metallic femoral component. Therefore, the contact pressure
module PressureModule was calculated from equations (3) to (5) as a function of the contact pressure \( p \)

\[
\text{PressureModule} = \frac{pA}{dA} = \frac{2p_o}{(1 + \nu)(1 - 2\nu)h} \left[ \frac{1}{c_0} + n \left( \frac{p}{p_o} \right)^{a-1} \right] \quad (6)
\]

where \( A \) is the unit contact area. Due to the range of the contact pressure over the articulating surface of UHMWPE tibial inserts from 5 to 25 MPa during a gait cycle, the maximum, minimum, and average PressureModule values corresponding to the contact pressure values were calculated as 2.59e11 N/m³, 0.48e11 N/m³, and 1.24e11 N/m³ respectively. Similar values for the PF joint were also adopted. The effect of using different PressureModule values on the model prediction was investigated.

**Inverse dynamics modeling**

Experimental ground reaction forces (GRFs) and marker trajectories were imported into the AnyBody MSK modeling system to calculate muscle forces and contact forces using a given muscle recruitment criterion typical for inverse dynamics analysis. In brief, the inverse dynamics modeling has two steps: first, kinematical model parameters are optimized to minimize the differences between model markers and the measured marker trajectories, which utilize a set of Karush–Kuhn–Tucker optimality conditions. The model scaling, local marker coordinates, and model motion during a dynamic trial are simultaneously optimized via the optimization routine. The pelvis and hip angle as well as foot spatial location are calculated during the kinematics optimization. Second, once optimized kinematics is derived, inverse dynamics analysis with a given muscle recruitment criterion is performed. Three muscle recruitment criteria were considered, including quadratic polynomial, cubic polynomial, and MinMax. The differences between the muscle recruitment criteria were described in the literature (also shown in Table 3). The calculated hip angles and foot spatial location were applied as inputs for actuating the MSK TKR model to simulate normal gait. Finally, the internal motion of TF, muscle activations, medial and lateral TF contact force, and PF contact force were derived from the combination of the GRF, segments mass, optimized muscle forces, and ligament action using the FDK solver in dynamics analysis. A normal gait cycle was simulated with a default time step of 282, and different time steps were also examined.

<table>
<thead>
<tr>
<th>Model parameters</th>
<th>Parameter description</th>
<th>TF_medial RMS</th>
<th>TF_medial ( R^2 )</th>
<th>TF_lateral RMS</th>
<th>TF_lateral ( R^2 )</th>
<th>PF RMS</th>
<th>PF ( R^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Analysis step</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Default value</td>
<td>The analysis step number between Start and End time adapting to the C3D file</td>
<td>46.50</td>
<td>0.97</td>
<td>39.16</td>
<td>0.97</td>
<td>35.99</td>
<td>0.99</td>
</tr>
<tr>
<td>Default value ( \times 2 )</td>
<td></td>
<td>59.14</td>
<td>0.99</td>
<td>17.90</td>
<td>1</td>
<td>27.95</td>
<td>0.99</td>
</tr>
<tr>
<td>Default value ( \times 0.5 )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Scaling law</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Length</td>
<td>Scale bone in three dimensions proportional to the length</td>
<td>40.85</td>
<td>0.99</td>
<td>23.78</td>
<td>0.99</td>
<td>15.65</td>
<td>1</td>
</tr>
<tr>
<td>Length–Mass</td>
<td>Scale bone in two directions according to the masses and one according to the length</td>
<td>12.21</td>
<td>0.99</td>
<td>19.27</td>
<td>0.99</td>
<td>6.48</td>
<td>1</td>
</tr>
<tr>
<td>Length–Mass–Fat</td>
<td>Scale as Length–Mass and consider the effect of fat percentage on muscle strength</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Muscle recruitment criterion</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Quadratic polynomial</td>
<td>Distribute the load between several muscles in various polynomial forms with power 2</td>
<td>72.08</td>
<td>0.99</td>
<td>54.34</td>
<td>0.96</td>
<td>17.98</td>
<td>1</td>
</tr>
<tr>
<td>Cubic polynomial</td>
<td>Distribute the load more evenly between muscles in various polynomial forms with power 3</td>
<td>57.02</td>
<td>0.99</td>
<td>46.29</td>
<td>0.97</td>
<td>15.84</td>
<td>1</td>
</tr>
<tr>
<td>MinMax</td>
<td>Distribute the collaborative muscle forces in such a way that the maximum relative muscle force is as small as possible</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>PressureModule</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Max 2.59e11 N/m³</td>
<td>The value corresponding to the contact stress of 5 MPa</td>
<td>41.39</td>
<td>0.99</td>
<td>26.30</td>
<td>0.99</td>
<td>17.03</td>
<td>1</td>
</tr>
<tr>
<td>Min 0.48e11 N/m³</td>
<td>The value corresponding to the contact stress of 25 MPa</td>
<td>50.47</td>
<td>0.98</td>
<td>37.89</td>
<td>0.98</td>
<td>19.27</td>
<td>1</td>
</tr>
<tr>
<td>Average 1.24e11 N/m³</td>
<td>The average value corresponding to the contact stress from 5 to 25 MPa</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

RMS: root mean square; TF: tibiofemoral; PF: patellofemoral.

More details on parameter description of the model can be found in AnyBody manual.

*The nominal value for investigating the effect of model parameters on knee contact forces by the RMS errors (N) and \( R^2 \) coefficients.
Results

Parameter sensitivity analysis

The sensitivity of the present computational model to the variation of the input parameters and different input models was examined first. Table 3 summarizes the predictions of medial and lateral contact forces of the TF joint and the PF contact force by root-mean-square errors (RMSEs) and correlation coefficients ($R^2$) for different input parameters. It is clear that the predicted contact forces were rather insensitive to the changes in these input parameters. Therefore, the default time step of 282, Length-Mass-Fat scaling law, MinMax muscle recruitment criterion, and average PressureModule value were adopted in the subsequent analyses.

Contact force

Once the numerical validation of the present model was performed, the predicted TF contact forces at the medial and lateral condyles are compared with the in vivo experimental measurements (Figure 2). Overall, good agreement between the predicted results and the experimental measurements can be observed, in terms of both the magnitude and the general trend. Particularly, for the medial contact force, an approximate error of 40 and 320 N was found at the two peaks corresponding to the early- and late-stance phases. While prediction error was increased for the lateral contact force in which three peaks were predicted with an approximate error of 299, 181, and 115 N, respectively, during a gait cycle. In general, the TKR computational model could predict medial contact force (RMSE = 215 N, $r = 0.96$), lateral contact force (RMSE = 179 N, $r = 0.75$), and total compressive force (RMSE = 344 N, $r = 0.95$) of the TF joint with a reasonable level of accuracy. In addition, the predicted patellar contact force and PCL force are also shown in Figure 2.

Muscle activation

Majority of the muscle activities predicted from the present computational model are consistent with the measured transformed EMG measurements in Figure 3. In particular, biceps femoris long head, semimembranosus, vastus lateralis, medial gastrocnemius,
lateral gastrocnemius, soleus, and gluteus maximus were predicted with a similar trend. However, prediction error was increased for the vastus medialis, tensor fasciae latae, and gluteus medius with different trends.

Joint motion
The internal motion of the TF joint in all three translational directions and three rotational directions was calculated using the FDK solver (Figure 4). In vivo

Figure 3. Comparison of measured and estimated muscle activations of the TKR patient during a normal gait.
flexion–extension, internal–external, and varus–valgus angles of femoral rotation with respect to the tibial insert ranged from 6.93° to 62.02°, −0.70° to 3.32°, and −0.25° to −1.08°, respectively. Meanwhile, the anterior–posterior, inferior–superior, and medial–lateral translations of the femoral component with respect to the tibial insert ranged from 3.90 mm to 0.06 mm, 2.77 mm to 0.98 mm, and −0.97 mm to −1.86 mm, respectively. The predicted femoral internal–external rotation had a peak internal rotation angle at 46% of gait cycle corresponding to the lowest flexion in the middle of the stance phase. The predicted peak anterior–posterior translation occurred at the beginning of the stance phase and the end of the swing phase.

Discussion
A dynamics model was developed in this study to predict contact forces, muscle activation, and joint internal motion simultaneously in the knee joint during normal gait by integrating a lower extremity MSK model implanted with a TKR. This enabled the consideration of the articular surface geometry and the deformation of the knee implant, dynamic skeletal models, and muscles and ligaments at the same time. To the authors' knowledge, no previous full lower extremity MSK TKR models with an explicit deformable articular contact model have been applied to compare the predicted TF contact forces and muscle activations against direct in vivo measurements, as well as to compute the internal motion of non-conforming knee implants, PF contact force, and PCL ligament force simultaneously during normal gait.

Four main potentials are presented in this research. First, compared with the traditional MSK models in which the knee was represented as a revolute joint, the model in this study considered 6 degrees of freedom, the geometry of the artificial knee implant, and the ligaments for a more realistic prediction of the TF and the PF contact forces. This is important since more realistic knee joint models could reduce the errors associated with skin marker–based kinematics measurements of TF motion than the idealized joint constraints for knee utilized in previous studies.36

Second, the majority of previously reported MSK models that took the geometry of artificial knee implants into account or encompassed elastic foundation contact models, for example, in Lin et al.’s study,9 only the knee joint is considered and other neighboring joints in the lower extremity are neglected. In fact, most muscles of human lower limb are crossing the knee as well as the ankle or the hip. Compared with those, the model in this study established a full lower extremity MSK model with the explicit articular contact geometry and considered the force-producing constraints imposed on the muscles from the neighboring joints as well as even the influence from the opposite knee. The medial and lateral contact forces of the TF joint, PF contact force, joint internal motions, ligament force, and muscle activations could be predicted simultaneously. Although Stylianou et al.18 also established a full lower extremity MSK model with the contact geometry of a TKR, the medial and lateral contact forces of TF joint and PF contact force were not reported, and only the squat and toe rise motions were simulated.

Third, fluoroscopy methods have been developed recently to examine the in vivo knee kinematics. However, the fluoroscopy measurements were difficult for different overground gait trails like turning-right gait. However, the model in this study could be applied to simulate more gait patterns for prediction of in vivo knee kinematics.

Finally, this study considered and presented more details of the modeling approach than the previous study by Andersen and Rasmussen,19 especially regarding the determination of the material parameter PressureModule, and the direct validation in terms of the contact force and muscle activation. In this study, a
realistic non-linear elastic material property PressureModule for the UHMWPE tibial insert was determined, with an average value of $1.24 \times 10^7 \text{N/m}^3$, while the previous study did not provide such information.

It is important to carry out a quantitative research of the contact forces that are closely related to TKR wear and loosening.\textsuperscript{37} The predicted medial, lateral, and total TF articular contact forces in this study are generally in good agreement with the measurements from the instrumented knee implant during normal walking gait. However, the muscle redundancy problem under inverse dynamics condition and inaccurate muscle moment arms (e.g. due to inaccurate muscle attachment points) or muscle-tendon parameter values may have led to the overestimation of the predicted tibial contact forces. The present model also estimated the PF contact force between the patella button and the femoral component. The predicted maximum PF contact force of 650 N falls in the range of 400–800 N reported by Ward and Powers\textsuperscript{38} under normal gait. The PCL ligament force was also reported in this study, which had one peak value of approximately 0.7 times body weight, which also falls in the range of 0.5–1 times body weight reported from the literature.\textsuperscript{39} However, caution must be exercised on these comparisons since different subjects and different conditions are involved.

For precise knowledge of in vivo implant biomechanical environment, articular motion is a key parameter to influence TKA functional performances. Quantitative understanding of in vivo total knee arthroplasty (TKA) kinematics remains a challenge.\textsuperscript{40} It is difficult to combine the capture of fluoroscopic data with the gait measurements of joint motions and force plate.\textsuperscript{41} This study demonstrated that the developed MSK TKR model was able to predict the in vivo TKA kinematics during normal gait. Although the in vivo knee motion was not available for the present subject, the predicted femoral motions were in reasonable agreement with previous literatures\textsuperscript{42,43} in terms of general trends (Figure 4). Especially, the predicted anterior–posterior translation and the predicted internal–external rotation show a similar trend to those of the measurements\textsuperscript{42} from a passive patient group where the right knee was replaced by the same implant type addressed in this study. The discrepancy in the amplitude may result from different gait patterns and patient factors.

Although the MSK TKR model developed in this study provided an opportunity for estimating in vivo knee internal motion, contact forces, and muscle activation simultaneously, this study still possessed a number of limitations. First, the origin and insertion sites of the muscles in the MSK TKR model were based on the generic TLEM model rather than the realistic patient-specific model. This may have resulted in a larger error in the predictions of the activity of some muscles and the lateral knee contact force. Only the muscle-fiber length was scaled by the scaling law, and the other force-producing properties of the muscles and the related parameters were not adjusted to consider the age and physical stature of the patient. Meanwhile, some muscles were divided into multiple branches in AnyBody MSK model, and the EMG signal was more related to the activity in part of a large muscle group closest to the electrode. This may contribute to large differences of some muscle activations. Moreover, the properties assigned for the ligaments in the model were obtained from the literature. Each ligament origin and insertion point was adjusted manually to fit with the bone geometry of the patient knee model according to the anatomic descriptions. The stability of ligaments and muscles plays an important role in inverse dynamic analyses so that the prediction may be affected by these approximations. Third, only a single gait trial from a single subject was adopted. Further investigation should involve more subjects and various activities for better assessment of the modeling system. Future studies should also consider the direct validation of the internal motions of the knee joint during gait cycles. Despite these limitations, the present model could offer a robust virtual modeling platform for pre-clinical assessment of knee implant designs, surgical guidance, and post-operative rehabilitation.

**Conclusion**

This study applied a novel FDK method for MBD analysis and considered the details of the modeling approach and the predictions of the medial and lateral compressive forces, joint internal motions, and muscle activations simultaneously in the knee joint during normal gait, in which a full lower extremity MSK model was combined with a subject-specific deformable TKR model. The comparison of the estimated TF contact forces/muscle activations with those from experimental measurements demonstrated the effectiveness of the current MSK TKR model to predict in vivo dynamics of the implanted knee joint with a reasonable accuracy.

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**Declaration of conflicting interests**

The authors declare that there is no conflict of interest.

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References

15. Mihalko WM and Williams JL. Total knee arthroplasty kinematics may be assessed using computer modeling: a feasibility study. Orthopedics 2012; 35: 40–44.
30. Cripton PA. Compressive characterization of ultra high molecular weight polyethylene with applications to contact stress analysis of total knee replacements. MSc Thesis, Queen’s University, Kingston, ON, Canada, 1993.
36. Andersen MS, Benoit DL, Damsgaard M, et al. Do kinematic models reduce the effects of soft tissue artefacts in


