

# SURROGATE-BASED CONTACT MODELING FOR EFFICIENT DYNAMIC SIMULATION WITH DEFORMABLE ANATOMIC JOINTS

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## INTRODUCTION

Knowledge of *in vivo* muscle, ligament, and joint contact forces can be valuable for studying issues related to neural control, rehabilitation, degenerative joint disease, surgical planning, and orthopedic implant design. Since these quantities are difficult to measure *in vivo*, dynamic musculoskeletal models are frequently used to develop predictions [1]. Muscle force predictions have been shown to be highly sensitive to the amount of constraint present in the assumed joint models [2]. For example, by constraining varus-valgus rotation, a pin joint knee model may alter predicted muscle forces by eliminating the need for muscles to stabilize this degree of freedom. Ligament force predictions are sensitive to the detailed kinematics of the joint. Since muscle co-contractions and ligament forces have an important influence on joint contact forces, constraint-based joint models also limit one's ability to predict *in vivo* joint contact forces accurately.

The ideal situation would be a dynamic musculoskeletal model where each anatomic joint was modeled as deformable using its surface geometry and material properties. The main problem with this approach is computational speed. For example, explicit finite element models of an artificial knee can take hours or even days of CPU time to complete a one cycle dynamic simulation [3,4]. More recently, dynamic knee simulations utilizing elastic foundation contact models have reduced computation time to 10 minutes [5,6]. However, even 10 minutes is problematic for optimization studies that perform repeated dynamic simulations of the musculoskeletal system. A new method is needed that permits multiple joints throughout the body to be modeled as deformable without increasing computational cost significantly.

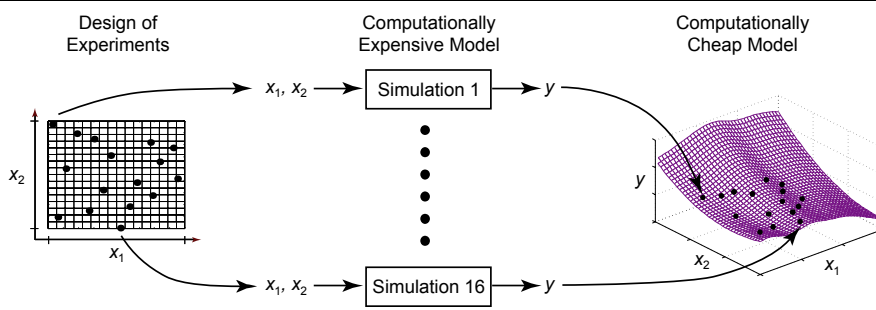
This study proposes a novel approach for speeding up dynamic musculoskeletal simulations containing deformable joint contact models. The concept involves replacing a computationally-costly geometry-based contact model (e.g., finite element or elastic foundation) with a computationally-

cheap surrogate contact model constructed from data points generated by the original model. An initial implementation is demonstrated using a dynamic simulation of a three-dimensional (3D) artificial knee model constrained to planar motion. Contact forces, joint motion, and CPU time determined using an elastic foundation contact model are compared to those found using a surrogate contact model.

## METHODS

A 3D multibody dynamic contact model was constructed for a cruciate-retaining total knee replacement (Series 7000, Stryker Howmedica Osteonics, Inc, Allendale, NJ). Dynamical equations were derived for the femoral component moving in the sagittal plane with respect to a fixed tibial insert. Sagittal plane rotation (i.e.,  $\theta$ ) was prescribed while superior-inferior (SI) translation (i.e.,  $y_{trans}$ ) and anterior-posterior (AP) translation (i.e.,  $x_{trans}$ ) were predicted by numerically integrating the equations of motion using the stiff solver `ode15s` available in Matlab (The Mathworks, Natick, MA). The prescribed flexion angle and applied loads in the SI and AP directions were taken from a planar version of a dynamic simulation performed in a previous study using the same implant model [5].

Contact loads applied to the femoral component and tibial insert (equal and opposite) were included in the dynamic simulation using two different deformable contact models. The first one was an elastic foundation (EF) contact model employing a fine element grid of  $50 \times 50$  on the medial and lateral sides of the tibial insert. The second one was a surrogate contact model created from sample points generated by the elastic foundation contact model. The goal was to determine whether a dynamic simulation performed with the surrogate contact model could closely reproduce the SI and AP motions and contact forces produced by the EF contact model but with substantially reduced computational cost. For both contact models, the dynamic simulation was performed on a 2.8 GHz Pentium 4 PC.



**Figure 1:** Overview of the steps involved in the surrogate model creation process. Sample points in design space are determined using statistical techniques from design of experiments (left). An analysis is performed with the computationally costly model at each of the specified design points (middle). The input-output relationship of interest is fitted with a computationally cheap surrogate model (essentially a multi-dimensional surface) (right) which can then be used in place of the original computationally costly model.

Development of the surrogate contact model involved four steps: 1) Design of experiments, 2) Computational experiments, 3) Surrogate model selection, and 4) Surrogate model evaluation (Fig. 1). Design of experiments is a statistical method for determining which locations in the input variable space (xtrans, ytrans, and zrot) should be sampled for predicting outputs of interest from the computationally-costly model (Fx and Fy from deformable contact). The goal is to maximize the quality of the resulting surrogate model fit while minimizing the number of sample points. Since contact forces are highly sensitive to changes in ytrans, we chose a 10 x 10 uniform grid of xtrans and zrot values whose extremes were determined by the limits of “realistic” motions. At each location on the grid, 9 sample points were generated by performing a static analysis with the EF contact model for loads varying from 10 to 4010 N in 500 N increments. Initial attempts to use statistical sampling methods that varied xtrans, ytrans, and zrot together proved unsuccessful since random sampling in the ytrans direction produced only a sparse number of points in contact.

Several surrogate model formulations were evaluated to fit the 900 sampled values of Fx and Fy as a function of xtrans, ytrans, and zrot. Kriging and polynomial response surfaces did not provide sufficient accuracy for dynamic simulation. However, when ytrans was plotted as a function of xtrans and zrot for any constant value of Fy (e.g., 10 N), smooth surfaces were produced. Thus, for each of the 9 known values of Fy, a 2D interpolating spline model was created to predict ytrans as a function of xtrans and zrot. An identical approach was used to predict Fx as a function of xtrans and zrot for each value of Fy.

Each time the dynamic simulation required a value for Fx and Fy, the surrogate contact model used the current values of xtrans, ytrans, and zrot to perform the following calculations. First, 9 new values of ytrans and 9 values of Fx were calculated from the 18 2D spline models using xtrans and zrot as inputs. Next, the resulting Fy-ytrans and Fy-Fx data points were fitted with a cubic interpolating spline. Finally, Fy was calculated from the Fy-ytrans spline curve using the current value of ytrans, while Fx was calculated from the Fy-Fx spline curve using the value of Fy just calculated.

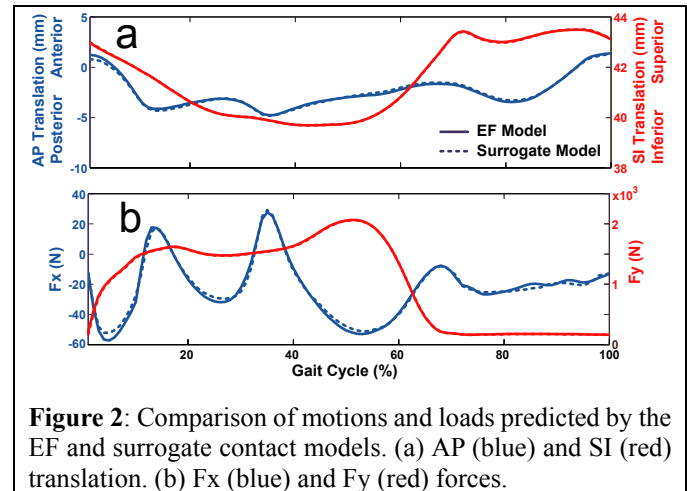
## RESULTS

The dynamic simulation that used the surrogate contact model closely reproduced the motions and loads predicted with the EF contact model (Fig. 2). However, motion and force were matched more closely in the SI direction than in the AP direction. While the dynamic simulation using the EF contact model required 28 minutes of CPU time, the simulation using surrogate contact model required less than a minute and a half.

## DISCUSSION

Fitting a computationally-cheap model to data points generated by a computationally-expensive possesses several advantages. First, generation of sample points for surrogate model construction requires repeated static rather than dynamic analyses. Second, the density of the contact element grid only affects the surrogate model creation process and has no effect on surrogate model run-time cost. Though a denser contact element grid will produce more accurate results with the EF contact model, the increase in computational cost can be

substantial. For example, a contact element grid of 100 x 100 requires 74 minutes of CPU to perform the same dynamic simulation. Third, multiple surrogate contact models can be embedded within any larger dynamic musculoskeletal model without incurring a large increase in computational cost. Though surrogate models could be used to fit the input-output relationships of an entire dynamic simulation, that approach is problematic due to fitting of a high-dimensional design space, plus any changes to the system being optimized would require costly new simulations to regenerate the surrogate models.



**Figure 2:** Comparison of motions and loads predicted by the EF and surrogate contact models. (a) AP (blue) and SI (red) translation. (b) Fx (blue) and Fy (red) forces.

The primary limitations of this approach are that the surrogate contact models must be regenerated for any changes in surface geometry or material properties. Also, friction effects are not included in this initial formulation. Because the current surrogate model was implemented using built-in Matlab functions, the 2D spline models were re-fitted each time a value of Fx and Fy was needed by the numerical integrator, significantly increasing the computational cost unnecessarily.

## CONCLUSIONS

This paper has presented a computationally efficient surrogate modeling technique for efficient dynamic simulation of musculoskeletal models with multiple deformable joints. In the sample knee replacement simulation, the surrogate contact model produced comparable accuracy with orders of magnitude improvement in computational speed. Refinement of the methodology for 2D problems and extension of the approach to 3D problems are topics for future research efforts.

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