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A Data-driven Surrogate Model to Connect Scales between Multi-domain Biomechanics Simulations

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***Abstract*—A data driven surrogate was developed to bridge the gap between finite element and multibody modeling and to expand the information available from a rigid multibody cartilage simulation. An indentation experiment performed on canine stifle cartilage was modeled in both paradigms with acceptable accuracy and the data were used to create the surrogate. Neural networks were found to adequately approximate the von Mises stress calculated by the finite element model based on force values provided from the multibody model with a correlation coefficient over 0.96.**

***Index Terms*— knee, canine, cartilage, multiscale, finite element, multibody**

I. Introduction

KNOWLEDGE of in vivo knee loading and cartilage stress would greatly benefit the development of engineered musculoskeletal tissues, joint injury prevention and repair, and our understanding of degenerative joint disease, specifically osteoarthritis. With current technologies, mechanical loading in the natural knee cannot be measured during dynamic activity. Computational techniques coupled with gait measurements and medical imaging hold the promise of predicting subject-specific joint loading. In general, two approaches are used in computational biomechanics; the finite element (FE) method and the multibody (MB) method. The finite element method can predict the internal stress and deformation of tissues, but simulations are computationally intensive, have simplified loading and boundary conditions, and typically do not include representation of individual muscles. The multibody method is used in body level musculoskeletal models that can predict individual muscle forces, but typically these models have simplified representations of the joints [1]. The overall goal of this work is to develop a multiscale modeling method that translates loading on rigid elements in a body level multibody musculoskeletal model to tissue-level prediction of stress (Fig. 1). Specifically, data-driven surrogate models that learn from cartilage level FE solutions will be embedded within an anatomical knee model placed in a body-level musculoskeletal model. The end result is concurrent prediction of muscle forces and tissue-level cartilage stress during forward dynamic simulations of movement.

Finite element models of articular cartilage are typically formulated from isolated cartilage with properties (and validation) determined through indentation, confined compression, or unconfined compression testing [2]. In vivo characterization of tissue-level parameters, such as stress, would benefit from inclusion of patient-specific joint loading, patient-specific geometries, and ideally, patient-specific material properties. FE tissue models have been coupled with musculoskeletal models to predict tissue-level stress in the patello-femoral joint [3, 4]. A limitation of these models is that they are not linked through concurrent simulation where tissue level parameters could influence muscle activations, which in turn would modify tissue-level loading. Halloran et. al. have used adaptive surrogate modeling techniques to couple the multibody and FE domains [5]. In their method a 2-D musculoskeletal model of jumping was coupled with a FE model of the foot. At each time step, a FE simulation was run or previous results utilized if a solution already existed within a user-specified tolerance.

Presented here is a method to develop a data-driven surrogate that learns from FE solutions of cartilage. The surrogate can then be embedded in MB musculoskeletal models for concurrent prediction of tissue level parameters. Specifically, various linear and non-linear models were developed to predict the von Mises stress of rigid cartilage elements in a MB model. Inputs to the surrogate models were reaction forces on the rigid cartilage elements and outputs were the resulting tissue level stress. Solution sets for surrogate training and validation came from MB and FE models of simulated indentation testing of canine tibia cartilage.

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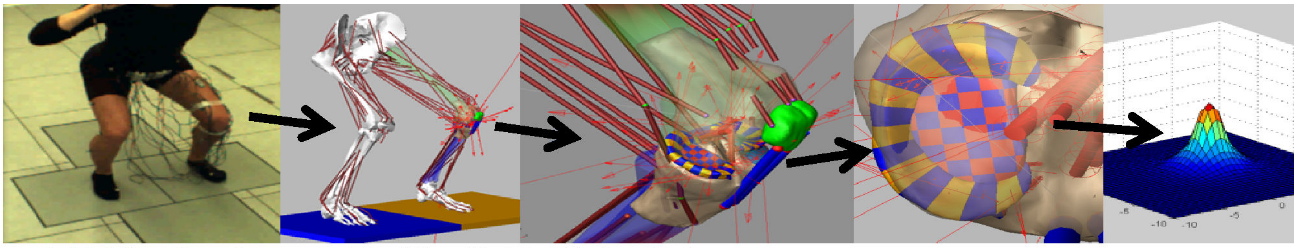

Figure 1: Modeling scheme for concurrent simulation of body-level to tissue level.

Experimental indentation tests were used to determine material properties for the FE model. The resulting surrogate increases the utility of MB models by increasing the amount of information that can be obtained, in this case by predicting von Mises stress.

II. Methods

A. Multibody Cartilage Overview

Multibody cartilage models can be created in the MD.ADAMS software (MSC software, Santa Ana, CA) from an IGES geometry of the articular cartilage through the use of custom ADAMS macros. These macros automate the process of intersecting a square prism with the cartilage geometry to generate a single segment that is then fixed to a part representing the underlying subchondral bone. Before moving to the adjacent space to repeat the process the macro creates a contact between the each new segment and the overlying part. The deformable contact law is a penalty function that discourages overlap:

$$F = K\delta^{e} + B(\delta)\dot{\delta} \qquad (1)$$

Where K is the linear stiffness, δ is the interpenetration depth, B is a damping coefficient and e is a force exponent. With appropriate tuning this contact law can be used to model many physiological loading scenarios (Fig. 2).

B. Experimental Validation

To first ascertain suitable properties for the MB and FE models a cartilage indentation experiment was performed. The experiment used a 2 mm radius impermeable indenter under a ramp force profile to determine the displacement of the articular cartilage of a canine tibial plateau. The indentation was performed approximately normal to the surface of a thawed specimen.

An FE model of the experiment was created using ABAQUS (ABAQUS Inc., Providence, RI) in order to determine the properties of cartilage. The tissue was represented by a cylinder of radius 20 mm and thickness 4.5 mm. The top layer, with a thickness of 2.14 mm (as measured from the MRI of a canine knee), was defined as cartilage and the bottom layer was defined as bone. The indenter was represented by a cylinder with a hemispherical tip of radius 2 mm. The cartilage and bone were defined as elastic solids; while, the indenter was modeled as a rigid shell with a steel equivalent point mass. The cartilage was meshed using 11445 hexahedral elements with a side length of 0.7 mm. Initial values for the material properties were determined from a previous study [6].

Dynamic explicit analysis was performed using this model. The general contact method was used to define the interaction between the cartilage and indenter. This method allowed definition of the contact between all regions of the model with a single interaction. It is generally used in cases of all-inclusive surfaces that contain external faces and shell perimeter edges. Normal interaction with hard contact was used to define the pressure overclosure. The indenter was constrained in all degrees of freedom except the vertical. The bottom surface of the cylinder was fixed in all degrees of freedom. A force matching the experimental load was applied to the indenter and the corresponding displacement was compared to the experimental value. The elastic modulus was tuned in this manner until a value of 32.5 MPa was determined to match the indenter displacement to the experimental values.

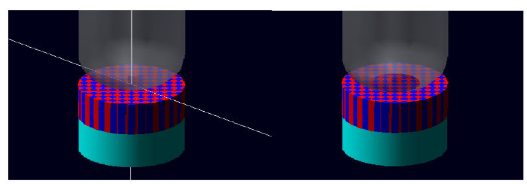

Figure 2. The calibration model in unloaded and loaded conditions showing the contact patch in the MB model.

For easier comparison between the models the cylindrical tissue in the above model was replaced by a cuboid of sides 20 mm and thickness 2.14 mm representing the cartilage. A total of 6400 hexahedral elements of side 0.5 mm were used to mesh the tissue. The bottom surface of the cuboid was fixed, all the other definitions were the same as above. The displacement of the indenter in this model was the same as that of the earlier model, so it was assumed that the cuboid with its bottom surface fixed could be used to represent the bone and cartilage in all the following models (Fig. 3 and 4).

The first MB model was created in MD.ADAMS and consisted of a 2.36 mm thick squat cylinder representing the underlying cortical bone, the MB cartilage, and the 2 mm radius spherical ended indenter (Fig. 2). The cartilage disc was partitioned using 0.5 mm square prisms. The measured force profile was applied along the vertical axis of the indenter and the corresponding displacement of the model was recorded. Design of experiments was used to modify the contact parameters to match the model displacement profile to that of the experiment. Specifically, three-factor central composite designs (CCD) were used to minimize the error between the two curves. The same load profile was used to determine appropriate FE model parameters.

C. Model Training Data Generation

To generate data that were more physiologically relevant, it was decided to use a 6 mm radius indenter and a dynamic loading profile that included sliding as well as vertical motion.

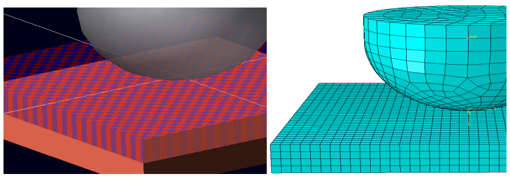

Figure 3. The MB training data model and the FE model.

The data extracted from ADAMS consisted of the location and reaction forces in the X, Y, and Z directions at a loaded segment and the reaction forces at the adjacent 4 segments. The data extracted from ABAQUS consisted of the reaction forces and the von Mises stress. Once the surrogate methodology was selected the final training data were collected from a model with a noisy profile. The noisy loading profile was driven by force in the vertical direction and by position in the lateral directions. The vertical force profile consisted of a ramp from 0-5 s and a constant level for the remaining 5 s. Low frequency noise was added to this, spanning from 1-10 s. The lateral position profile similarly consisted of a ramp and hold with noise and a maximum displacement of 5 mm. Noise was added to the lateral profile from 5-10 s and the lateral profile was applied at a random angle between 10-35°.

D. Surrogate Creation

Both linear and nonlinear surrogate models were explored to find the functional relationship between the von Mises stress from the FE model and the reaction forces from the MB model, which to our knowledge has never been characterized. For nonlinear system identification, several single hidden layer feed forward neural networks (NN) were investigated. NNs have been shown to be universal nonlinear function approximators [7], and thus it is hypothesized that their regression is better than linear regression models, which have been used as the reference point in this study.

Mean squared error (MSE) was chosen as model performance measure, which is calculated as the average of the squared differences between model-predicted vs. desired (ground truth) outputs. The choice of MSE for fitness metric was further corroborated by observation of zero-mean, Gaussian residues of the NN models (Fig 5). It can be shown that the maximum likelihood solution for regression, if successful, leads to minimizing the MSE when modeling errors have normal distribution [8]. Additionally, correlation coefficients between model predictions and desired outputs, R, are also reported (Fig. 6). The closer the R-values to one, especially for the unseen test data, the better. Furthermore, smaller disparities between training and test performance measures are a sign of proper training and appropriate choice of model, as over-parameterized models tend to have low training but high test errors [9].

All the models were simulated using 64 bit MATLAB®, version R2010b (Mathworks, MA) and its neural network toolbox running on an Intel® Core-2 Duo® based computer with 64 bit Mac OS X® 10.6 operating system.

Linear Regression: For the linear surrogate, a 15-dimensional linear model was fit to 70% of the data chosen by random selection as the training set. The remaining 30% was used to test the model, yielding a training MSE of 1,625,700 kPa^2 and a test MSE of 1,660,700 kPa^2. The predicted vs. target correlation coefficients were 0.6916 for training and 0.6847 for test data Obviously the linear surrogate was not successful in capturing the system's input-output relationship given its poor performance, in terms of high MSE and low R, on both test and training data.

Neural Networks: Given the dependence of learning and generalization power of NN models on their size [9], 15 different neural networks with 2-30 nodes in their hidden layers were examined, where the number of nodes in their hidden layers was varied from 2 to 30. Hyperbolic tangent activation functions were chosen for the hidden nodes. Linear activation functions were used for the output nodes to achieve larger dynamic range and better performance [9]. Levenberg-Marquardt gradient decent algorithm was used with validation based early stopping to preserve the generalization power of the trained networks. The dataset was partitioned into training (70%), validation (15%), and test (15%) subsets using random sampling. The results for each NN were averaged over five training runs starting from randomly initialized weight sets, as NNs may converge to a different local solution during each iterative gradient descent solution.

Among the investigated NNs, the best model size was chosen using two criteria for better generalization: lower validation error, and smaller size. The result was a network with 16 hidden nodes yielding average training MSE of 97,397 kPa^2, average validation MSE of 108,630 kPa^2, and average test MSE of 108,260 kPa^2.

III. Results and Discussion

The overall results have closely followed the expected trends. The FE and MB models were able to reproduce experimental conditions (Fig. 4) and an NN-based surrogate modeling method was identified. This is supported by the blind testing of another 5 s loading profile in all models. This produced the expected error distribution (Fig. 7).

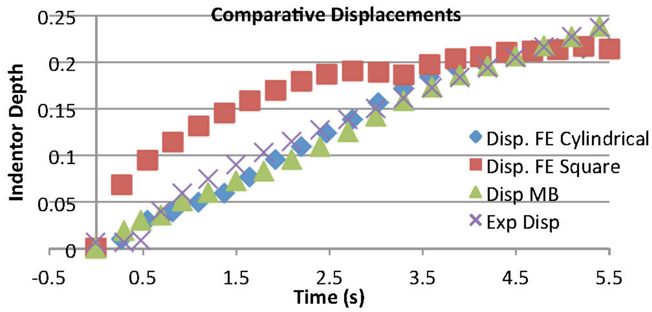

Figure. 4: Comparative displacements of the two FE models, the MB model and the experimental displacements.

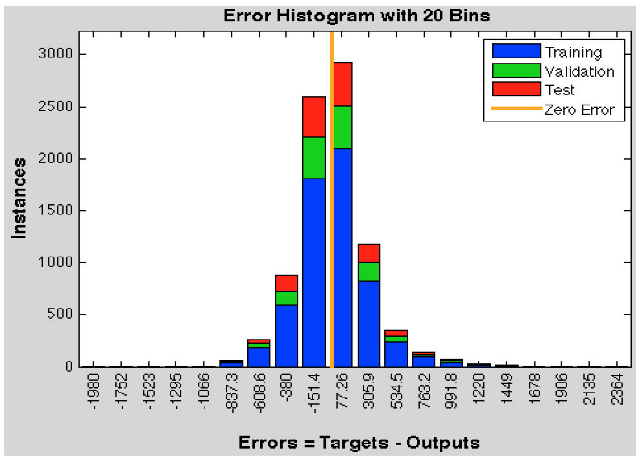

Figure. 5: Sample error distributions of a 16-node, 1 hidden layer neural network model showing an almost zero-mean Gaussian distribution over its modeling residues.

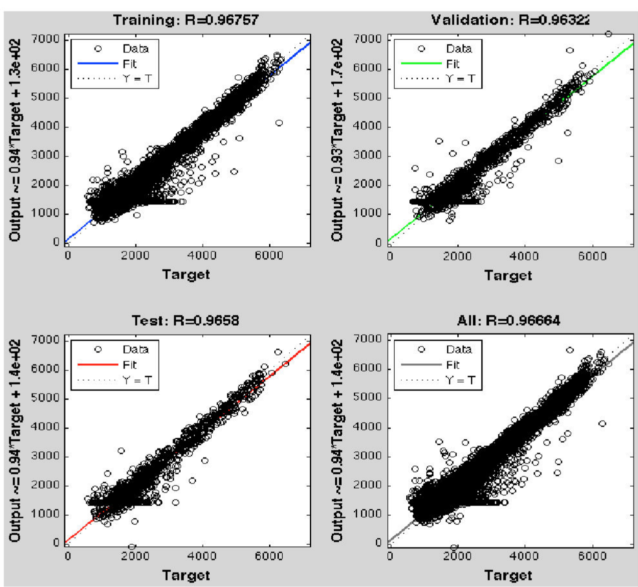

Figure. 6: Correlation plots for a sample 16-hidden node neural network model (best configuration).

A feed forward NN with 16 hidden nodes produced errors that were at least 14 times better than the linear surrogate. Figure 6 also shows significantly better correlation coefficients between NN predictions and ground truth, with R being larger than 0.96 over training, validation, and test datasets. The small disparity between training and test fits, along with nearly zero mean Gaussian distribution of the errors (Fig. 5), are further indications of successful NN modeling.

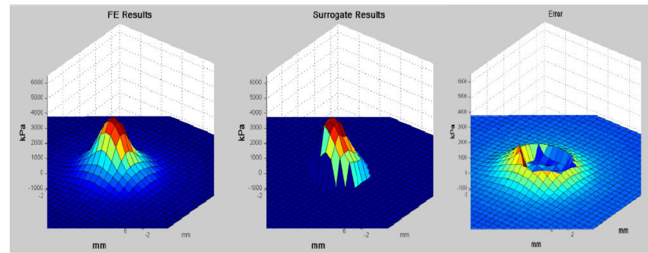

Figure 7. Von Misess stress and the error of the surrogate at 2.5 s.

The overall inadequacy of linear models and the success of NN surrogate models was expected from previous work using surrogates to model joint kinematics [10]. While these are both biological models, they focus on different physical outputs. However, both datasets were well fitted by NN's leaving zero-mean Gaussian errors, supporting the choice of NNs as nonlinear data-driven surrogate models for biomechanical simulations.

IV. Conclusion

It has been shown that a joint level MB model can accurately predict tissue level stress by training a surrogate model on a detailed tissue level FE model. While the models used in this study consisted of simplified geometries and model parameters, they demonstrate that it should be possible to use accurate anatomical limb level models to estimate tissue stress.

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