Multiobjective Design Optimization of Total Knee Replacements Considering UHMWPE Wear and Kinematics

by

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A thesis submitted to the
Department of Mechanical and Materials Engineering
in conformity with the requirements for
the degree of Doctor of Philosophy

Queen’s University
Kingston, Ontario, Canada
April 2010

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Abstract

Total knee replacement is the gold standard treatment for restoring mobility and relieving pain associated with osteoarthritis when other medical therapy has failed. Revision surgery is necessary when the replaced knee fails, which is often a result of implant damage (such as wear) or poor kinematics.

Design optimization is a method for finding the best shape for a component using an optimization approach considering one or multiple performance metrics. The shape of a parametric candidate design can be manipulated by an optimization algorithm, which seeks to minimize an objective function subject to performance constraints and design space limitations. During multiobjective design optimization, multiple performance measures are minimized simultaneously, the relative importance of each determined using a weighted sum. This approach can also be used to derive a Pareto curve or frontier which graphically describes the relationships (or trade-offs) between the performance measures.

It was hypothesized that a trade-off exists between wear and kinematics performance in total knee replacements. The objective of this research was to test this hypothesis by using multiobjective design optimization to describe this relationship
with a Pareto curve. It was first necessary to develop and validate numerical frameworks for wear and kinematics simulations, using models constructed using a parametric modeller. The Pareto curve was then generated using a combination of single objective and multiobjective design optimizations considering these two performance measures.

Single objective optimization for wear yielded a theoretical design with superior wear resistance when compared to a typical commercially available knee design. Single objective optimization for kinematics yielded a theoretical design capable of higher flexion, as well as more natural laxity characteristics. After performing multiobjective design optimization, the resulting Pareto curve showed that there is, in fact, a trade-off between wear and kinematics performance. When considering optimum designs, in order to improve the wear performance it was necessary to sacrifice kinematics performance, and vice-versa. This previously suspected but never verified nor quantified relationship can be used to improve total knee replacement designs, as well as help healthcare providers select the best implants for their patients.
Acknowledgments

I’d like to start by acknowledging the support and guidance of my supervisor, Dr. Il Yong Kim. You’ve kindled my interest in academic research, and I’ve learned more than a few research survival skills from you. I can’t thank you enough for seeing the potential in me and our research and for encouraging me to switch into a Doctoral program. It took a little bit longer than originally intended, but the end product has been well worth the wait.

I’d also like to thank all of the past and present Structural and Multidisciplinary System Design (SMSD) lab members. I could not ask for a better set of co-workers and friends to share an office with. It is remarkable how a group of students working on completely different research topics are able to provide so much help and support to one another. I wish the best to all of you in whatever paths you choose.

I also have to thank the staff and faculty of the Mechanical and Materials Engineering department, from the main office to the shop floor. You are the gears that keep this machine running and able to produce the strong students and innovative research that this school is known for.

By far, one of the biggest benefits of doing my undergraduate and doctoral studies at Queen’s has been the close proximity to friends and family. It is impossible to thank you enough for how much you’ve helped me survive school. My friends provided an
escape from my research when I needed a break. Whether I met you in University, High School or Kindergarten, you’ve all helped me reach my full potential. I’m absolutely positive I would have cracked before my thesis defense if not for the support and encouragement of those closest to me.

Finally my family – the most loving and supportive people in the world. Your encouragement and patience has been unwaivering. Mom, I hope enough of your English skills made it to me and are reflected in my writing. Dad, the technical skills you passed on to me are the only reason I was able to finish my experiments on time. Andrew and Laura – best siblings ever. I can’t believe we used to fight over car seats and slices of pizza. I don’t know of any other family that has as much fun together as we do. You make Kingston home. I love you all.
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<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>AA</td>
<td>Adduction / abduction</td>
</tr>
<tr>
<td>AAOS</td>
<td>American Academy of Orthopaedic Surgeons</td>
</tr>
<tr>
<td>ABS</td>
<td>Acrylonitrile butadiene styrene (ABS plastic)</td>
</tr>
<tr>
<td>ACL</td>
<td>Anterior cruciate ligament</td>
</tr>
<tr>
<td>AMTI</td>
<td>American Mechanical Technologies, Inc</td>
</tr>
<tr>
<td>AP</td>
<td>Anterior / posterior</td>
</tr>
<tr>
<td>ASTM</td>
<td>American Society for Testing and Materials</td>
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<tr>
<td>CAD</td>
<td>Computer aided design</td>
</tr>
<tr>
<td>CIHI</td>
<td>Canadian Institute for Health Information</td>
</tr>
<tr>
<td>CJRR</td>
<td>Canadian Joint Replacement Registry</td>
</tr>
<tr>
<td>CoCr</td>
<td>Cobalt-chrome (CoCr alloy)</td>
</tr>
<tr>
<td>CR</td>
<td>Cruciate-retaining</td>
</tr>
<tr>
<td>CS</td>
<td>Cross shear (ratio)</td>
</tr>
<tr>
<td>DOF</td>
<td>Degree of freedom</td>
</tr>
<tr>
<td>EDTA</td>
<td>Ethylenediaminetetraacetic acid</td>
</tr>
<tr>
<td>FE, FEM, FEA</td>
<td>Finite element, FE method, FE analysis</td>
</tr>
<tr>
<td>HHT</td>
<td>Hilber-Hughes-Taylor (integrator)</td>
</tr>
<tr>
<td>IE</td>
<td>Internal / external</td>
</tr>
<tr>
<td>iRed</td>
<td>Infrared marker</td>
</tr>
<tr>
<td>ISO</td>
<td>International Organization for Standardization</td>
</tr>
<tr>
<td>LCL</td>
<td>Lateral collateral ligament</td>
</tr>
<tr>
<td>MCL</td>
<td>Medial collateral ligament</td>
</tr>
<tr>
<td>ML</td>
<td>Medial / lateral</td>
</tr>
<tr>
<td>MPC</td>
<td>Multi-point constraint</td>
</tr>
<tr>
<td>nRMS</td>
<td>Root mean square, normalized to range of measurement</td>
</tr>
<tr>
<td>OA</td>
<td>Osteoarthritis</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
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<tr>
<td>--------------</td>
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<tr>
<td>PCL</td>
<td>Posterior cruciate ligament</td>
</tr>
<tr>
<td>PFC</td>
<td>Press fit condylar</td>
</tr>
<tr>
<td>PMO</td>
<td>Predominant molecular orientation</td>
</tr>
<tr>
<td>RMS</td>
<td>Root mean square</td>
</tr>
<tr>
<td>STL</td>
<td>Standard tessellation language</td>
</tr>
<tr>
<td>TKR</td>
<td>Total knee replacement</td>
</tr>
<tr>
<td>UHMWPE</td>
<td>Ultra high molecular weight polyethylene</td>
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Table 2: Symbols related to wear modelling

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$q_i$</td>
<td>Tangential force during substep $i$</td>
</tr>
<tr>
<td>$s_i$</td>
<td>Sliding distance vector during substep $i$</td>
</tr>
<tr>
<td>$\theta_i$</td>
<td>Sliding direction during substep $i$</td>
</tr>
<tr>
<td>$\bar{\theta}$</td>
<td>Predominant molecular orientation (PMO)</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Amount of crossing motion</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Fraction of fibrils aligned with PMO (strain hardened)</td>
</tr>
<tr>
<td>$W_\perp$</td>
<td>Frictional work perpendicular to $\bar{\theta}$</td>
</tr>
<tr>
<td>$W_\parallel$</td>
<td>Frictional work parallel to $\bar{\theta}$</td>
</tr>
<tr>
<td>$W_{tot}$</td>
<td>Total frictional work</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Coefficient of friction</td>
</tr>
<tr>
<td>$K$</td>
<td>Material specific wear parameter (specific to frictional work model)</td>
</tr>
<tr>
<td>$k$</td>
<td>Wear parameter (in reference to Archard’s wear model)</td>
</tr>
<tr>
<td>$\delta_{aligned}$</td>
<td>Wear damage of fraction aligned with PMO</td>
</tr>
<tr>
<td>$\delta_{multi}$</td>
<td>Wear damage of multidirectional fraction</td>
</tr>
<tr>
<td>$\delta_{wear}$</td>
<td>Total wear damage depth</td>
</tr>
</tbody>
</table>

Table 3: Symbols related to creep modelling

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C'$</td>
<td>Compressive creep compliance</td>
</tr>
<tr>
<td>$\delta, \lambda, \eta$</td>
<td>Creep model curve parameters</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
</tbody>
</table>
Table 4: Symbols related to fatigue damage modelling

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D$</td>
<td>Fatigue damage score (higher = damage more likely)</td>
</tr>
<tr>
<td>$S_i$</td>
<td>Shear stress at turning point</td>
</tr>
<tr>
<td>$i$</td>
<td>Turning point (shear stress increasing to decreasing, or opposite)</td>
</tr>
<tr>
<td>$T$</td>
<td>Number of turning points</td>
</tr>
</tbody>
</table>

Table 5: Symbols related to kinematics modelling

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi$</td>
<td>Average Y-axis values (forces, torques) within a given X-axis range (displacements, rotations)</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>Highest Y-axis value within a given X-axis range</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Lowest Y-axis value within a given X-axis range</td>
</tr>
<tr>
<td>$\epsilon_s$</td>
<td>Slope or stiffness error</td>
</tr>
<tr>
<td>$\epsilon_f$</td>
<td>Hysteresis or friction error</td>
</tr>
<tr>
<td>$\epsilon_{tot}$</td>
<td>Overall error between two data sets</td>
</tr>
<tr>
<td>$\mu_{static}$</td>
<td>Static coefficient of friction</td>
</tr>
<tr>
<td>$\mu_{dynamic}$</td>
<td>Dynamic coefficient of friction</td>
</tr>
</tbody>
</table>

Table 6: Symbols related to design optimization

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\bar{x}$</td>
<td>Candidate design vector</td>
</tr>
<tr>
<td>$x_{min}$</td>
<td>Lower bound for design vector</td>
</tr>
<tr>
<td>$x_{max}$</td>
<td>Upper bound for design vector</td>
</tr>
<tr>
<td>$J(\bar{x})$</td>
<td>Performance of candidate design</td>
</tr>
<tr>
<td>$C_{eq}(\bar{x})$</td>
<td>Equality constraint status of candidate design</td>
</tr>
<tr>
<td>$C(\bar{x})$</td>
<td>Inequality constraint status of candidate design</td>
</tr>
<tr>
<td>$\nabla J(\bar{x})$</td>
<td>Gradient of performance about candidate design</td>
</tr>
<tr>
<td>$w$</td>
<td>Weighting factor - relative importance of multiple $J(\bar{x})$</td>
</tr>
<tr>
<td>$W_{vol}$</td>
<td>Volumetric wear after 3.5 million cycles of simulated wear</td>
</tr>
<tr>
<td>$\delta_{max}$</td>
<td>Maximum total damage depth after 3.5 million cycles of simulated wear</td>
</tr>
<tr>
<td>$D_{max}$</td>
<td>Maximum damage score after 3.5 million cycles of simulated wear</td>
</tr>
<tr>
<td>$J_{wear}$</td>
<td>Wear objective function</td>
</tr>
<tr>
<td>$\text{flex}_{max}$</td>
<td>Maximum safe flexion angle</td>
</tr>
<tr>
<td>$\text{err}_{tot}$</td>
<td>Overall error in implant constraint versus natural knee</td>
</tr>
<tr>
<td>$\text{err}_0$</td>
<td>Error in implant constraint about laxity neutral point, versus natural knee</td>
</tr>
<tr>
<td>$\text{var}_{pcl}$</td>
<td>Percentage change in maximum safe flexion by adding / removing PCL</td>
</tr>
<tr>
<td>$J_{kin}$</td>
<td>Kinematics objective function</td>
</tr>
<tr>
<td>$J_{MOO}$</td>
<td>Objective function for multiobjective design optimization</td>
</tr>
</tbody>
</table>
Chapter 1

Introduction

1.1 Motivation

Arthritis is a condition suffered by more than four million people in Canada [1]. Affecting approximately one in six Canadians, arthritis is a leading cause of pain and physical disability [1]. The number of Canadians suffering from arthritis is expected to reach six million by the year 2026 [1]. Osteoarthritis (OA) is a form of arthritis where inflammation of the joints is caused by wearing of articular cartilage. Patients experience pain upon weight bearing during activities such as walking, stair climbing or standing, and a tendency to limit motion may lead to regional muscle atrophy and ligaments becoming more lax.

In severe OA of the knee, loss of articular cartilage causes pain, swelling, stiffness, loss of mobility, and in general, a reduced quality of life. Where medical therapy can no longer adequately control the progression of OA of the knee, the gold standard treatment is total knee replacement (TKR), which provides pain relief and improved mobility. A TKR involves removal of the badly damaged articular cartilage and
subchondral bone at the distal femur and proximal tibia. The surfaces are replaced with implanted components which normally consist of a metal femoral component, tibial tray and an ultra high molecular weight polyethylene (UHMWPE) bearing insert. Depending on the condition of the patella and the design of the implant, an UHMWPE component usually replaces the contact surface of the patella as well.

The most recent annual report from the Canadian Joint Replacement Registry (CJRR) by the Canadian Institute for Health Information (CIHI) reported 37,943 hospitalizations for knee replacement in 2006 (excluding Quebec) [2]. Comparing to 15,829 reported 10 years earlier in 1996, the frequency of TKR has more than doubled (140%), and an increase of 9% compared to the report in 2005. A study presented to the American Academy of Orthopaedic Surgeons (AAOS) in 2006 projected US TKR primary implantation rates to increase from 450,400 in 2005 to almost 3.5 million by 2030 (if implantations continue at current rates). The CIHI also reported that the most notable increases in knee replacement rates were seen in the 45 to 54 age groups, lowering the mean patient age for TKR (68.6 years in 2004). Younger, more active patients would place higher demands on TKR components, and require greater implant longevity.

If the primary TKR is not successful, a revision surgery is necessary. Revision involves the adjustment, addition or replacement of one or more implant components. Revision procedures are generally considered a greater risk for patients because of longer surgery times (to remove the failed components and repair damaged tissues) and the removal of more natural bone stock. Revision also poses an economic burden, due to the expense of a second surgery which is generally more expensive than the first (see Table 1.1). In Canada, revision surgery accounts for approximately 6% of
hospital visits for knee replacement, reporting 2,641 in 2006 (excluding Quebec) [2], and the rate in Canada is lower than reported by several other countries (see Table 1.2). In 2004, the most common reasons for TKR revisions in Canada were reported as aseptic loosening (35%), UHMWPE wear (30%), osteolysis (17%) and infection (13%) (Fig. 1.1) [3]. In 2006, these numbers changed slightly to aseptic loosening (25%), UHMWPE wear (17%), infection (16%) and instability (14%) [2]. Figure 1.2 shows that revision, if necessary, normally occurs close after primary surgery, with nearly 50% of revisions occurring within 11.5 months [4]. A study of 212 TKR revisions by Sharkey et al. [5], however, found that wear was the most prevalent reason for TKR revision, and the average time from primary to wear-related procedures was approximately 7 years.

Table 1.1: Average cost of primary and revision TKR procedures by country, in USD (revised from [6]). Average revision costs all exceed those of the primary TKR procedure in that country.

<table>
<thead>
<tr>
<th>Country</th>
<th>Year</th>
<th>TKR</th>
<th>Revision TKR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Australia</td>
<td>2004</td>
<td>$11,543</td>
<td>$16,789</td>
</tr>
<tr>
<td>Canada</td>
<td>2005</td>
<td>$7331</td>
<td>$8850</td>
</tr>
<tr>
<td>England/Wales</td>
<td>2004</td>
<td>$9263</td>
<td>$10,670</td>
</tr>
<tr>
<td>New Zealand</td>
<td>2003</td>
<td>$7101</td>
<td>$8537</td>
</tr>
<tr>
<td>Sweden</td>
<td>2005</td>
<td>$11,582</td>
<td>$15,960</td>
</tr>
<tr>
<td>United States</td>
<td>2003</td>
<td>$15,476</td>
<td>$16,006</td>
</tr>
</tbody>
</table>

1.2 Limitations in TKR Design

A revision rate of 6% is too high considering the number of TKR procedures and the forecasted increases in the years to come. The design of the implant used during TKR factors largely into the success or failure of the joint replacement [7]. While
CHAPTER 1. INTRODUCTION

Figure 1.1: Reasons for TKR revisions in Canada in 2004–2005 and relative frequency of each [3].

![Reasons for TKR revisions](image1)

Note: Percentages do not add up to 100% as more than one reason for revision can be recorded.

Figure 1.2: Percentage of revised knee replacements in Canada from July 2001 to March 2006, as a function of time (in months) from the primary surgery [4].

![Percentage of revised knee replacements](image2)

Source: Canadian Joint Replacement Registry. Canadian Institute for Health Information, July 2001 to March 2006.
Table 1.2: Percentage of TKR procedures which are revisions, by country (revised from [6]).

<table>
<thead>
<tr>
<th>Country</th>
<th>Crude Revision Rate (Percent)</th>
<th>Year</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Australia</td>
<td>9</td>
<td>2004</td>
<td>National Joint Replacement Registry</td>
</tr>
<tr>
<td>Canada</td>
<td>6</td>
<td>2003</td>
<td>Canadian Joint Replacement Registry</td>
</tr>
<tr>
<td>England/Wales</td>
<td>4</td>
<td>2004</td>
<td>National Joint Registry for England and Wales</td>
</tr>
<tr>
<td>New Zealand</td>
<td>9</td>
<td>2004</td>
<td>New Zealand National Joint Register</td>
</tr>
<tr>
<td>Sweden</td>
<td>7</td>
<td>2004</td>
<td>Swedish Knee Arthroplasty Register</td>
</tr>
<tr>
<td>United States</td>
<td>8</td>
<td>2003</td>
<td>American Academy of Orthopaedic Surgeons</td>
</tr>
</tbody>
</table>

Preoperative patient specific and surgical factors and postoperative rehabilitation also contribute to the outcome of the procedure, the design of the implant will ultimately limit how well the replacement can perform.

Wear of the UHMWPE bearing component in TKR and unnatural implant kinematics are often cause for TKR revision. Worn components will not be able to function as designed, and significant wear alone can be cause for revision. The wear debris released into the joint space can also be the cause for revision. The debris can trigger an adverse tissue reaction known as osteolysis, which will lead to implant loosening. Current TKRs are unable to fully restore natural knee kinematics, which may also lead to revision. The natural knee provides a certain amount of stability for standing and the stance phase of gait. Instability in TKR is often cause for revision. The range of motion in TKR is often limited by the lack of femoral rollback, a motion
seen during natural knee flexion which is necessary for allowing deep flexion. The feasibility of a TKR design is determined by its ability to satisfy both wear related and kinematics related performance requirements.

A wide variety of different TKR designs have been developed, but the most common design by far is the condylar total knee replacement. Why this design is so common is a function of its resemblance to the natural knee, previous clinical success, and the high costs associated with developing innovative new implant designs. We also tend to see that most condylar designs are very similar, with similar radii of curvature shared by different designs and essentially symmetric condyles. TKR design has departed from the natural knee here, which normally has asymmetric condyles with complex curvature to properly distribute load and guide knee motion. This departure is necessary due to the limitations of the materials we have to use in TKRs, and to compensate for soft tissues removed during surgery. The question that still remains is – how do we possibly know that we have the best condylar TKR design? Without doing any rigorous investigation of the entire spectrum of possible condylar TKR designs, it is possible that we are reusing less than optimal designs which are limiting the success of TKR \textit{in-vivo}.

Development and refinement of TKR is a slow process due to the complex requirements of the joint. Wear testing of a single implant design will take approximately two months. Numerous experiments with the same design should be performed to give the results some statistical significance, which requires the development and destruction of many prototypes. To perform a parameter study on all of the different features of a TKR design is made infeasible. The same is true for studying implant kinematics: prototypes must be developed and lengthy experiments must be performed. On top
of this, we do not know the sensitivity of a TKR design to soft tissue characteristics, surgical procedure and other patient specific variables without clinical trials.

Numerical modelling and computation play a more important role in the design cycle than ever before, because they allow us to evaluate many different designs with relative ease when compared to experiments in-vitro and the following clinical trials. They allow us to screen out the best designs from the rest and push those along to further research and development, rather than rely on previous results and know-how in selecting what designs to move forward with. While previous experience and know-how are still extremely important in the design process, they may cause designers to make assumptions about certain designs which could have easily been evaluated at little cost through numerical approaches.

Despite the widespread use of computers in TKR design, we still do not see highly numerical automated design methods being used for these components. More importantly, there has not been an in-depth study of TKR designs in order to find the optimum three-dimensional shape considering both wear and kinematics performance. Without such study, we do not know if the standard TKR shape is close to the optimum, or if there is much room for improvement. We also do not know if there is any trade-off between wear performance and kinematics performance. The only way to truly develop an optimum design is to consider all important performance measures and constraints simultaneously.

1.3 Objective

The global objective of this work is to use multiobjective design optimization to simultaneously consider UHMWPE damage and implant kinematics while finding the
optimum TKR shape. Using a numerical approach and gradient based optimization methods, it will be possible to efficiently examine the TKR design space to find the best TKR design. By varying the relative importance of wear performance versus kinematics performance, it is possible we will find that the different performance measures are both sensitive to the same design features, but in fact might have conflicting relationships. This is very common, and two performance measures which are related to one another in such a way are called competing performance measures. In order to improve with respect to one performance measure, it often requires a sacrifice in terms of another performance measure.

Several sub-objectives must also be met to facilitate TKR multiobjective design optimization. These include:

1. Development and validation of a numerical framework for wear simulation.

2. Development and validation of a numerical framework for kinematics simulation.

3. Development of a parametric modelling framework to allow simulation of any candidate TKR shape.

4. Single objective design optimization for wear and for kinematics in order to determine both optimum shapes.

5. Multiobjective design optimization considering wear and kinematics simultaneously.

For multiobjective optimization to be possible, appropriate computational frameworks for wear (sub-objective 1) and kinematics (sub-objective 2) simulations must be developed and validated, because experimentally measuring implant performance
is prohibitively expensive and time consuming. These simulations must be capable of assessing the performance of any condylar TKR design which is presented to them, and must always return reliable and accurate results.

The designs will be provided to the simulations in the form of a three-dimensional virtual model. Therefore, a computational framework must also be built to generate these three-dimensional models (sub-objective 3). Modelling code will receive a vector of design instructions which describe the shape of the candidate TKR design, and will build the three-dimensional model from those instructions.

Combining the parametric modeller with the wear or kinematics simulation frameworks and selecting an appropriate performance measure (objective function) will permit single objective design optimization (sub-objective 4). Design optimization considering wear or kinematics alone will determine what design traits are most desirable for either objective function. These optimizations will also help determine the anchor points for a Pareto curve derived using multiobjective optimization.

A Pareto curve describes the relationship between two, potentially competing, performance measures. The end points (anchor points) of this curve are generally determined using single objective optimization, but the shape of the curve between these end points must be determined using multiobjective optimization (sub-objective 5).

Meeting each sub-objective is a necessary step towards the global objective of determining the relationship between TKR wear and kinematics, described with a Pareto curve. The results will also determine the optimum TKR shape in terms of wear and kinematics, and simulation frameworks for both performance measures will be validated.
1.3.1 Hypothesis

Based on the findings of Sathasivam and Walker [8], it is hypothesized that there is a trade-off between wear and kinematics performance. The natural knee requires a certain amount of laxity to allow natural kinematics. The constraint at the natural knee is provided predominantly through soft tissue contributions. Since the soft tissue balance is altered during TKR, the contact surface of the implant components must provide constraint instead. This limits the laxity of the replaced knee. It is also believed that high surface conformity is required at the implant contact surface in order to minimize contact stresses. High contact stresses can lead towards material failure or wear problems for UHMWPE. It is believed that the laxity requirements of the natural knee can not be fully satisfied while maintaining a design which also fully addresses the conformity requirements for minimal UHMWPE damage. While there is most likely a trade-off between wear and kinematics performance, multiobjective design optimization will allow us to quantify this trade-off with a Pareto curve. This will allow us to select designs which give the best trade-off between the objective functions.

1.4 Contributions

Several contributions are described in this thesis. One of the biggest contributions is the numerical framework for the prediction of UHMWPE wear in TKR. A unique strain hardening sensitive UHMWPE wear model was developed in order to account for the sensitivity of UHMWPE wear to counterface crossing motions. The wear
model proposed is superior to any published UHMWPE wear models to date, combining very strong predictive capability while only requiring a single experimental parameter to be tuned. The wear model was tuned and validated with regards to a specific implant design, but can be extended to any metal-on-UHMWPE material pairing, such as total hip or shoulder replacements.

The kinematics simulation framework is another substantial contribution to the field of TKR simulation. The research showed that standard experiments for TKR laxity and flexion assessment can be simulated numerically with relative ease. This thesis also describes the use of ABS plastic implant prototypes versus typical implant materials. The results show that novel designs can be assessed through simulation and experiment without the need for prototypes fabricated from actual implant grade materials.

The most significant contribution and the focus of this research was the application of multiobjective design optimization to TKR. The extensively coded and validated computational framework combined with a powerful optimization algorithm allowed the quantification of the relationship between TKR wear and kinematics. The trade-off is described using a Pareto curve. This Pareto curve can be a very powerful tool for decision making at the design level, allowing one to input their own preference for TKR performance (wear or kinematics) while knowing exactly the sacrifice required in the other objective function. Thus, the designer can select an implant design which best satisfies their preference while maintaining an optimum design.


1.5 Organization of Thesis

Chapter 2 begins with a background of some of the numerical methods we use for simulation (finite element analysis and rigid body dynamic modelling). This is followed by background information on the natural knee and total knee replacement. In depth discussion of the background and previous work for TKR wear and kinematics research is also included in this chapter. An explanation of optimization and multiobjective optimization, and previous attempts at optimizing TKR follows.

Chapter 3 outlines the development and validation of a numerical framework to predict UHMWPE wear using finite element contact analysis.

Chapter 4 outlines the development and validation of a numerical framework to predict TKR kinematics using rigid body dynamics software.

Chapter 5 describes multiobjective design optimization of a total knee replacement considering wear and kinematics. The development of a parametric modeller and modifications to the wear and kinematics frameworks described in Chapters 3 and 4 are discussed, followed with single and multiobjective optimization results.

Chapter 6 summarizes the entire body of work and the relevance of the results. The success or failure to meet the individual sub-objectives described in Section 1.3 or the global objective of the thesis will be discussed here.

The Appendices contain some notes on experimental procedure and some results plots for reference which did not require placement in the main body. A more in-depth description of the numerical frameworks can also be found there.
Chapter 2

Background

2.1 Finite Element Analysis

The finite element method is used to find numerical solutions to complex problems in several engineering disciplines, including solid mechanics. This analysis method involves dividing a solid continuum into many smaller finite elements which are connected at nodes, called a finite element mesh. Rather than obtaining an analytical solution for the complex problem, solutions for each of the simple finite elements are obtained simultaneously which provide an approximate result to the complex problem. As the mesh is refined, the approximate solution approaches the true solution. In structural mechanics, this involves calculating the displacements at each node which will be a function of the loads, boundary conditions, and the stiffness of the elements connecting the nodes.

Finite element analysis is further complicated if contact between two parts is included. Nodes are not shared between the two parts, so different approaches must be used to transfer contact forces between the two. The Penalty or Augmented
Lagrange methods can be used in these situations. Special elements are used at the contact interfaces which together form a contact pair. One surface of the contact pair is capable of recognizing when it is being penetrated by the other contact surface. Penetration of one surface (the target surface) through the other (the contact surface) will apply a penalty to the total system energy, and the system will respond by generating contact forces to push the contact surface away from the target surface (causing deformation of the contact surface, the development of contact and internal stresses, and reducing penetration). This procedure repeats until the penalty has been reduced to an acceptable level. If the Augmented Lagrange method is used, the solver will also calculate the maximum penetration depth, and if the penalty criterion has been satisfied but the maximum depth criterion has not, the penalty stiffness will be increased and the penalty method iterations are restarted. This process iterates until convergence in terms of the penalty and maximum depth criteria are both satisfied. Generally speaking, the Augmented Lagrange method will provide a more accurate solution than the Penalty Method alone; however, results will depend on the specifics of the contact situation being analyzed.

Finite element analysis can be broken down into three processes. The first is pre-processing. This involves the generation of the finite element mesh (discretization). At this point, material properties, element properties, loads and boundary conditions are also selected. The next phase is the actual solve process. At this point, the solver routine performs calculations to determine the displacements at each of the nodes, and can use a number of different equation solver methods which are beyond the scope of this dissertation. The final step is post-processing, where results are interpreted, and displacements, stresses and other results data are extracted and
used for further processing (if necessary). Often, all of these processes are performed within the finite element analysis package, although software exists which can be used as a substitute to the built-in pre- or post-processing modules. An example is Altair\textsuperscript{TM} HyperWorks\textsuperscript{TM}, which can be used as a pre- and post-processor for finite element (FE) solvers like ANSYS\textsuperscript{TM}, despite it being distributed with its own pre- and post-processors.

2.2 Rigid Body Analysis

Rigid body dynamics packages are available which allow kinematic models to be developed, with part interactions generally handled by some sort of mechanical joint. Equations of motion for each part are generated and assembled into a set of non-linear equations and unknowns. Due to the number of unknowns, numerical methods are used to solve the equations of motion in real-time, and the rigid body displacements of parts can be tracked and recorded until a stable equilibrium point or simulation termination point is reached.

Rigid body dynamics analysis packages may also come with contact modelling capabilities. The contact can be modelled using similar methods as those used in FE analysis, except surfaces cannot deform and become stressed. Instead, only repellent contact forces are generated normal to the contact surfaces (and tangential if friction is included), based on the penetration of one contact surface into another. Unlike in FE analysis, the contact stiffness cannot be automatically determined by the program because it does not have material stiffness information, so users must define these values and validate their results.
2.3 Finite Element versus Rigid Body Analysis

Generally speaking, the finite element method calculates much more information than rigid body dynamics. Since parts are deformable, internal stress information is gathered which cannot be obtained using rigid bodies. The trade-off is computational expense. FE analyses often take an order of magnitude longer to yield a solution when compared to rigid body dynamics. This means that for simulations when deformations have negligible impact on the overall dynamics, and internal stress data is not required, rigid body dynamics is a desirable approach. If deformations carry significant impact on the final solution or internal stress data is required, it will be necessary to use the finite element method. An exception which should be noted is the ability of some rigid body dynamics packages to model flexible bodies. Flexible bodies must first have their mode-shape responses calculated within an FE package and can only rarely be used in contact, which means they cannot replace FE analyses for contact analysis.

2.4 The Natural Knee

What follows is a summary of the structure and motions of the natural knee joint. This is intended as a brief introduction, sufficient to provide the reader with enough background to understand the terminology discussed later in the text. Should the reader require a more in-depth description on the anatomy and function of the natural knee, I would refer them to the source for this section, Clinical Kinesiology and Anatomy by Lynn S. Lippert [9], or similar text. Some terminology used for explaining anatomical directions and planes are described in Figure 2.1 and Table 2.1.
The knee joint is the largest joint in the body and is classified as a synovial hinge joint, which means articulation between two cartilage articular surfaces lubricated by synovial fluid. Figures 2.2, 2.3 and 2.4 show the important bones and soft tissues at the knee. The knee has a predominant flexion-extension motion, normally from approximately 0 degrees extension to 120–135 degrees of flexion. Knee motion is complex, and as the knee flexes there is internal rotation of the tibia with respect to the femur coupled with a posterior displacement of the femur with respect to the tibia. The opposite occurs in extension until the knee reaches a locked position, enabling us to load the knee without requiring significant muscle contribution. These rolling, gliding and rotation motions are guided by the shape of the femoral and tibial condyles, the meniscus, ligaments and muscles.
Table 2.1: Description of the anatomical directions used for describing relative locations and anatomy of the human body.

<table>
<thead>
<tr>
<th>Term</th>
<th>Direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Medial</td>
<td>Towards midline of body</td>
</tr>
<tr>
<td>Lateral</td>
<td>Away from midline of body</td>
</tr>
<tr>
<td>Proximal</td>
<td>Toward a reference point</td>
</tr>
<tr>
<td></td>
<td>(usually toward torso)</td>
</tr>
<tr>
<td>Distal</td>
<td>Away from a reference point</td>
</tr>
<tr>
<td>Inferior</td>
<td>Lower or below</td>
</tr>
<tr>
<td>Superior</td>
<td>Upper or above</td>
</tr>
<tr>
<td>Anterior</td>
<td>Toward the front</td>
</tr>
<tr>
<td>Posterior</td>
<td>Toward the back</td>
</tr>
</tbody>
</table>

### 2.4.1 Bones at the Knee

The knee joint actually comprises two separate articulations. The tibiofemoral joint is the articulation of the femur against the tibia, and the patellofemoral joint is the articulation of the patella against the femur. The patella is a sesamoid bone within the quadriceps muscle tendon. This bone provides some protection to the anterior surface of the knee as well as providing an increased moment arm length to maximize the effectiveness of the quadriceps. While the fibula is sometimes associated with the knee, it provides little aside from an attachment point for soft tissues, and is more important to the ankle joint.

### 2.4.2 Cruciate Ligaments

The cruciate ligaments lie between the medial and lateral condyles, and cross each other obliquely (Fig. 2.4). The anterior cruciate ligament (ACL) attaches to the intercondylar area on the anterior surface of the tibia, just medial to the medial meniscus. This ligament spans the knee and attaches posteriorly on the lateral condyle.
CHAPTER 2. BACKGROUND

Figure 2.2: Depiction of the anatomy of the proximal tibia in the natural right knee, as viewed from a superior position [9]. The tibia is oriented such that the anterior surface of the knee is at the top of the figure.

of the femur. The posterior cruciate ligament (PCL) attaches to the intercondylar area of the posterior tibia and spans the knee on the medial side of the ACL. It attaches to the anterior femur on the medial condyle. The ACL prevents the femur from displacing posteriorly on the tibia, and tightens during extension to prevent knee hyperextension. The PCL, conversely, prevents anterior displacement of the femur on the tibia, and tightens to provide a greater contribution during flexion. Together, the cruciate ligaments are predominantly responsible for providing sagittal plane stability.

2.4.3 Collateral Ligaments

The collateral ligaments are located on either side of the knee and provide frontal plane stability (Fig. 2.2). The medial collateral ligament (MCL) is a flat, broad ligament which attaches to the medial femoral epicondyle and the medial tibial condyle. The lateral collateral ligament (LCL) is a round, cord-like ligament which attaches to the lateral femoral epicondyle and connects to the head of the fibula. The attachments of the collateral ligaments are offset posteriorly and superiorly to the axis of flexion,
which causes them to become slack during flexion, but tight during extension to contribute to knee stability.

### 2.4.4 Menisci

The medial and lateral menisci are located on the superior surface of the tibia and are wedge-shaped fibrocartilage disks. The menisci are concave shaped and deepen the relatively flat joint surface. The menisci help to guide the motions of the knee, provide shock absorption, provide a low friction surface for joint articulation and increase the contact area to provide lower contact stresses.
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Figure 2.4: Depiction of the natural knee, fully extended, from the sagittal plane [9]. Figure depicts the cruciate ligaments and the patella as well as the femur and tibia.

2.5 Total Knee Replacement

2.5.1 Implant Component Design

A myriad of different TKR implant styles have been developed and have reached different levels of clinical success. The modern TKR design which is comprised of multiple knee components can be traced back to the design described by Thermestocles Gluck in 1890 [10]. This was a modular design that formed a simple ivory hinge, capable of only the flexion-extension motion. The first non-hinged total knee replacement was designed and used by Canadian Frank Gunston during a stay with Sir John Charnley in 1968 [10]. The metal and polyethylene implant designs that we see today were inspired by his original design. The typical condylar total knee replacement consists of a femoral component, tibial tray, UHMWPE insert and often an UHMWPE patellar component. See Figure 2.5 from [11].

The femoral component (Fig. 2.6) is usually metal, often cobalt-chrome, although
Figure 2.5: Illustration of a typical right knee condylar TKR from an anterior/lateral point of view (left), and a left knee TKR (right) modified from [11]. Each consists of a femoral component, UHMWPE insert, tibial tray and UHMWPE patellar component.

Some ceramic designs have been investigated [12]. The condylar shape is similar to the natural shape of the femur, but usually quite simplified in comparison. A patellar groove along the anterior to distal surface of this component accommodates articulation with the natural or resurfaced patella. The femoral condyles extend from the distal surface, posteriorly, and are usually symmetrical. These condyles accommodate articulation against the UHMWPE bearing insert. All articulating surfaces of the femoral component are polished to a mirror finish, while the inside surface is left unpolished and often conditioned to improve bone ingrowth.

The UHMWPE insert (Fig. 2.7, left) generally traces the outline of the proximal tibia in the transverse plane, with a flat bottom and two dished out areas on the upper surface for articulation with the femoral condyles. The bottom edge normally has specialized shapes to help lock the UHMWPE insert into the tibial tray, although different implant designs have mobile bearings (Fig. 2.7, right) which can move with
Figure 2.6: Illustration of the femoral component of a typical right knee cruciate retaining condylar TKR, modified from [11].

respect to the tibial tray. The contact surfaces of the UHMWPE insert are smooth, and have a very low coefficient of friction against polished metal surfaces. This component is the weakest and most prone to failure in a TKR, and frequently the reason for TKR revision.

Figure 2.7: Illustration of an UHMWPE bearing insert component of a fixed bearing (left) and mobile bearing (right) condylar TKR, modified from [11].

The tibial tray (Fig. 2.8, left) is usually metal, often titanium, and is anchored into the proximal tibia. The primary function of the tibial tray is to provide a foundation for the UHMWPE insert, which normally snaps on to the tibial tray or articulates with its superior surface. Unless the component is designed for a mobile bearing (Fig. 2.8, right), the surface is not usually polished to a mirror finish. Backside wear caused by micromotion with respect to the tibial tray is a known contributor to UHMWPE wear debris generation, but to a much lesser extent than the femoral contact surface.
Figure 2.8: Illustration of a tibial component from a fixed bearing (left) and mobile bearing (right) condylar TKR, modified from [11].

The last component is the UHMWPE patellar component, which resurfaces the posterior surface of the patella for articulation with the groove on the femoral component. This component can be anatomically shaped or simply a dome-like shape, depending on the implant design. If the natural patella is in good condition and the implant design allows it, resurfacing might not be necessary. While this component is also made of UHMWPE and can wear, the patellofemoral joint is rarely reported as a significant source of wear debris in comparison to the tibiofemoral joint.

2.5.2 Procedure

The procedure for total knee replacement can take 1 to 3 hours depending on the condition of the knee at the time of surgery. In the most common approach, the surgeon will make an incision down the front of the knee, then flex the knee while allowing the patella to slide to the lateral side of the joint. This exposes the contact surfaces of the distal femur and proximal tibia. Some soft tissues are excised, including the menisci (which must be severed from the medial collateral ligament), the anterior cruciate ligament (ACL), and sometimes the posterior cruciate ligament (PCL) depending on its condition and the type of implant being used. Intramedullar and external guides are used to position cutting jigs which allow the orthopaedic surgeon...
to cut away the damaged articular cartilage and subchondral bone and shape the distal femur and proximal tibia for the replacement components. Bone spurs, which are usually present in badly arthritic knees, are clipped off. Once the surfaces have been prepared, the surgeon uses special sizing equipment and implant components to determine the exact implant size to use. Any necessary adjustments to the soft tissues and bone cuts are performed to ensure proper soft tissue balance in extension and flexion and mechanical axis alignment. Achieving a good soft tissue balance is critical to knee function after TKR, because a knee which is too tight or lax in flexion or extension will require revision. Implant components are installed, usually held in place with a layer of bone cement, and the incision is closed. The natural knee, the knee bones prepared for receiving implant components, and the installed components are depicted in Figure 2.9.

Figure 2.9: Illustration of TKR procedure on a right knee, modified from [13]. Natural knee depicted on the left, natural knee prepared for TKR in middle, and knee with TKR components installed on right.
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2.6 TKR Damage

The most commonly damaged component in TKR is the UHMWPE insert. Damage due to abrasive and adhesive wear, creep, and fatigue are discussed here. Other damage modes such as burnishing, scratching, and third-body wear are also known to damage the UHMWPE insert, and for more information the reader is referred to the seven commonly reported mechanisms for surface degradation described in [14].

2.6.1 UHMWPE Wear

Abrasive and adhesive wear of the UHMWPE component of TKRs is a major limitation to the long-term success of these devices [5, 15–18]. Wear debris is known to be one of the triggers for osteolysis (the active resorption or dissolution of bone tissue) at the bone-implant interface. It is believed that macrophages become activated by the presence of large numbers of submicron wear debris [15, 16, 18–20]. The submicron wear debris in TKR is also accompanied by occasional wear particles greater than 3 microns, which are engulfed by giant cells [15–18]. As osteolysis progresses, the bone supporting implant components degenerates into soft periprosthetic tissue, eventually leading to implant loosening and instability requiring revision surgery. Even neglecting osteolysis, heavily damaged UHMWPE components in TKR will require revision, due to loss of mechanical effectiveness or fracture and dislocation of bulk UHMWPE material.

Previous experimental work using pin-on-disk and knee simulators has revealed a very important characteristic of UHMWPE wear; that the wear rate is sensitive to the direction of counterface motion [21–29]. Polymer molecules form as long chains, and the chains intertwine and bond to one another. When external work is applied
(such as frictional work from a sliding counterface motion), the orientations of these molecules are manipulated, causing molecular reorientation to align with the predominant sliding direction [27–29]. This leads to a significant degree of strain hardening, which results in an increased wear resistance in that direction. Strengthening in one direction causes a weakening against wear in the transverse direction, known as orientation softening [27].

The wear resistance of UHMWPE can be improved by increasing the number of bonds between chains. Highly-crosslinked UHMWPE is becoming increasingly popular because of the promise of wear rates as much as an order of magnitude less than conventional UHMWPE [25, 30]. Unfortunately, crosslinking also results in decreases in some aspects of mechanical performance, such as toughness, modulus, ultimate tensile strength, yield strength, hardness [25] and creep [31].

2.6.2 UHMWPE Creep

Creep, or cold-flow, is the time-dependent deformation of a material subjected to stress. UHMWPE is a viscoelastic / viscoplastic material, which undergoes elastic and plastic deformations under load in a time-dependent manner [32, 33]. While this does not contribute to any wear debris generation, the progression of creep damage will affect the progression of wear, so both damage modes must be considered in TKR design [34]. By modifying the shape of the contact surface, creep damage can also affect implant kinematics. The ability to estimate the magnitude of creep damage in total joint replacements is also useful in measuring the progression of wear damage. Using radiographic methods, it is possible to measure the progression of UHMWPE damage in an implant [34]. If a creep model exists which can reasonably
estimate the expected creep damage based on typical loading and duration \textit{in-vivo}, and total damage can be measured, an estimate of the damage caused by wear can be calculated. Creep damage generally follows a logarithmic progression, with the most damage occurring early on during what is referred to as the “bedding-in” period of the implant.

### 2.6.3 UHMWPE Fatigue Related Damage

Cracking, pitting and delamination are also commonly observed damage modes at the contact surface of TKR UHMWPE inserts [35–37]. One of the biggest factors in these damage modes was oxidization, and advances in sterilization and packaging techniques has helped to greatly reduce these failures. It is also believed that sub-surface stress fluctuations below the contact surface can fatigue the material [38, 39], contributing to crack propagation and pitting / delamination. As the point of contact with the femoral component moves across the contact surface of the UHMWPE insert, the subsurface stresses can increase / decrease drastically, and often quickly shift from compressive to tensile. Unlike the abrasive/adhesive wear mechanism which produces bioactive submicron debris, this damage mode is most likely to cause more catastrophic damage to the UHMWPE components leading to revision, rather than aseptic loosening from osteolysis.

### 2.6.4 Previous Work

Simulating these TKR damage modes using computational approaches is of great interest due to the time and costs associated with experimental approaches. While simulations cannot replace the necessary \textit{in-vitro} testing required for new implant
designs (such as ISO 14243 [40, 41]), the number of prototypes tested at this stage can be reduced by effective in-silico pre-screening. A great deal of research has thus focused on the numerical simulation of different TKR damage modes.

Archard’s Wear Model

Metal-on-metal wear rates can be estimated if contact pressures, sliding distances, and a wear coefficient $k$ are known by applying Archard’s classic wear model [42] (Equation 2.1). The model is introduced here because, while originally formulated for estimating metal-on-metal wear rates, the model was found to be effective for predicting metal-on-UHMWPE wear rates. It should be noted that this model does not take sliding direction into account. The model offers no dependence on the direction of counterface motion, a now widely recognized property of UHMWPE.

$$\delta_{\text{wear}} = kPs$$

where:

$\delta_{\text{wear}}$ is the linear wear depth [mm]

$k$ is the contact specific wear coefficient [MPa$^{-1}$] \hfill (2.1)

$P$ is the contact pressure [MPa]

$s$ is the relative sliding distance [mm]

TKR UHMWPE Wear Modelling

Some of the earliest simulation work for wear of artificial joints was published by Maxian et al. [43], simulating abrasive / adhesive wear of the acetabular liner of THA.
Their approach used the finite element method to calculate the stress distribution and sliding distances across the contact surface during simulated gait loading. Archard’s classic wear model [42, 44] was used to estimate wear. Later improvements to the model allowed the calculation of wear progression (to account for nonlinearities and material removal) using adaptive remeshing [45]. Selection of an appropriate wear factor \( k \) provided good agreement with experimental results. The model was then used for a parameter study of different femoral head sizes [46].

Researchers began using numerical methods to calculate UHMWPE contact stresses in TKR during simulated gait cycles using three-dimensional FE [47–52] and elastic foundation [53–55] models in the early 2000’s. The earliest TKR simulations which actually predicted UHMWPE wear using three-dimensional models were those of Fregly’s group at the University of Florida. Their original model used in-vivo walking and stair climbing kinematic data [53, 56]. Using a rigid body elastic foundation model, they calculated wear using Archard’s classic wear model [42, 44] and creep using the model published by Lee and Pienkowski [33]. Using \( k \) values from the literature, good agreement with retrieved specimens was observed.

The most important parameter in Archard’s wear model is \( k \), and many inconsistent values have been reported in the literature [57]. Generally speaking, good agreement between a simulation using Archard’s wear model and corresponding experimental results of wear tests can always be yielded by adjusting the wear coefficient \( k \), giving it more of a fudge factor reputation rather than that of a meaningful material parameter.

Some authors have been able to use consistent \( k \) values and yield good results. A recent model by Zhao et al. [58], a continuation of the work in Fregly’s lab, used a
$k$ value of 2.59E-07 mm$^3$/Nm that was determined experimentally using pin-on-disk testing with materials matching a commercially available implant design. Using this $k$ value for surface evolving TKR wear simulations, good agreement was seen with matching experimental results. Knight et al. [59] used an adaptive remeshing FE TKR wear simulation and Archard’s wear model to predict UHMWPE wear damage but not creep. Good agreement with experimental results was observed when using a literature derived $k$ value of 2.64E-07 mm$^3$/Nm.

The inability of Archard’s wear model to account for UHMWPE strain hardening offers an explanation of why so many inconsistent $k$ values have been reported. Without accounting for strain hardening, $k$ will be a function of not just the material properties and tribological conditions, but also the relative kinematics at the contact surface. At the contact surface of TKR, the counterface motion is generally unidirectional, which perhaps explains why some previous authors obtained acceptable results using consistent wear factors, but their models should fail under situations where more crossing motion is introduced.

Most of the more recent works in TKR wear simulation have included some means of accounting for crossing motions. One approach is to use the ratio of medial-lateral to anterior-posterior counterface motion to measure crossing motion and scale a constant wear factor [60]. The weakness of such an approach is the assumption that the motion is predominantly unidirectional in the anterior-posterior direction, which is not necessarily true at every point on the UHMWPE contact surface. Another method looks at the distribution of sliding vectors to quantify crossing motion and then calculate $k$ [61]. Unfortunately neither method relies on any theoretical derivation and instead have been fit to experimental observation.
Wang [28] published a unified theory for UHMWPE wear in multidirectional sliding which is based on the principle of frictional work, which was supported by pin-on-disk experimental work published by Turell et al. [22]. This model assumes polymer molecule reorientation in a preferred direction, called the predominant molecular orientation (PMO). Using pin-on-disk testing and the frictional work approach pioneered by Wang, Kang [23] developed a relationship to calculate $k$ at any point on an UHMWPE contact surface based on the local cross-shear ratio. This model was used for total hip replacement wear simulation incorporating cross-shear and contact pressure with very good agreement to experimental results [62]; however, performance under different kinematic conditions and TKR wear has not yet been demonstrated.

**UHMWPE Creep Modelling**

Lee and Pienkowski [33] published a creep model which has been used widely for UHMWPE creep damage in total knee replacements [56, 58, 63]. A more recent study by Lewis and Carroll [31], however, found that creep resistance is slightly reduced during crosslinking. While highly crosslinked UHMWPE is not yet widely used in TKR, the sterilization procedure does introduce some moderate crosslinking which would reduce creep resistance. Lewis and Carroll [31] published creep parameters (Equation 2.2) which are more appropriate for the modern, moderately crosslinked UHMWPE used in TKR today. To date, no published work by other researchers has used these updated material properties.
\[ C' = \delta + \lambda (\log t)^\eta \]

where:

- \( C' \) is the compressive creep compliance [\% MPa\(^{-1}\)]
- \( \delta = 0.0434 \)
- \( \lambda = 0.0715 \)
- \( \eta = 1.3956 \)
- \( t \) is time [s]

**Fatigue Damage Modelling**

Sathasivam and Walker [38] developed a fatigue damage model based on shear stress fluctuations in a finite element mesh of the UHMWPE insert of TKR. A damage function that estimates the susceptibility to subsurface cracking was defined as:

\[
D = \frac{1}{T} \sum_{i=1}^{T-1} |S_{i+1} - S_i| \times 0.5 \times \left( |S_{i+1}| + |S_i| \right)
\]

where \( S_i \) to \( S_T \) are the values at successive turning points on the graph of maximum shear stress for each element (see Fig. 2.10).

The highest damage score of all elements in the UHMWPE mesh was the representative damage score for that TKR design. The model was applied to two different TKR designs, which differed mostly in terms of frontal radii of curvature and frontal conformity. The damage score for the large radii, higher conforming design was three
times lower than the other, in agreement with the findings of several published retrieval studies. Other researchers studied sagittal conformity using a two-dimensional model using this approach, with similar fundings [39]. This method requires knowledge of the stress distribution within the UHMWPE insert, so rigid body elastic foundation models do not provide enough information to calculate the damage scores using this approach. No published examples have been found which consider both abrasive/adhesive wear and fatigue damage in the same model.

2.7 TKR Kinematics and Laxity

2.7.1 TKR Flexion Kinematics

During flexion of the natural knee, the femur displaces posteriorly with respect to the tibia. The posterior displacement of the lateral femoral condyle is greater, causing a
relative internal rotation of the tibia. This femoral translation is referred to as femoral rollback and is important for achieving deep flexion. Femoral rollback provides clearance for the poplital structures posterior to the knee and prevents bone-on-bone contact which would otherwise cause sublaxation at high flexion angles (Fig. 2.11). Femoral rollback is generally achieved through a combination of contact geometry and tensioning of the PCL during flexion.

Figure 2.11: Depiction of knee flexion without (top) and with (bottom) femoral rollback mechanism. During flexion, femoral rollback provides greater posterior clearance and prevents sublaxation.

The postoperative range of motion is an important determinant of patient satisfaction after TKA, and improvement in daily activities can be expected if a flexion arc of 110° or more is achieved [64]. In certain situations, greater flexion is required for floor activities, sports, and squatting positions [65]. The postoperative flexion range of motion after TKR is generally most sensitive to the preoperative range of motion [66, 67], although the importance of preoperative range of motion seems to only be a factor when it is too low [64].

Several authors have agreed that PCL retention after TKR can preserve rollback [68, 69]. While in-vitro studies with cruciate retaining TKR designs show femoral
rollback, it is not observed frequently during *in-vivo* studies [70]. Cruciate sacrificing TKR designs are also used. These designs feature a cam mechanism to force femoral rollback, but this mechanism reduces internal-external rotation laxity and is a potential site for wear and failure.

### 2.7.2 TKR Laxity

The laxity or constraint characteristics of a TKR are usually quite different from those of the natural knee. This is due to inherent differences in how constraint is provided in the two cases. In the natural knee, little constraint is provided by the knee geometry, and is instead provided by the soft tissues. In the replaced knee, however, the removal of the ACL greatly reduces AP constraint, which must instead be provided by the implant contact surface geometry [71]. This also causes the laxity of TKR to be very sensitive to the axial load, unlike the natural knee whose laxity is almost independent of axial load [71]. The correct amount of constraint in extension and flexion is necessary to the stability and range of motion of TKR, and should be reproduced as closely as possible, although this can pose wear and soft tissue strain issues [8, 72, 73].

Anterior-posterior (AP) laxity and internal-external (IE) laxity are the most often studied at the knee, and typical knee laxity values are shown in a paper by Li et al. [74]. Generally speaking, AP and IE laxity are both lower in extension than when flexed. This provides greater stability when the knee is fully extended, requiring less muscle activity for long term weight bearing. Laxity increases once the knee flexes to permit femoral rollback, internal rotation and other femorotibial kinematics.
CHAPTER 2. BACKGROUND

2.7.3 Previous Work

Much research has focused on simulating the natural knee using experimental and computational approaches. Simulating the natural and replaced knee has been attempted both experimentally and numerically. Numerical approaches have generated validated natural knee models, which are often used to better understand the contributions of different aspects of knee anatomy [74–84].

By far one of the most prolific research groups in TKR kinematics is that of Walker. In the mid 1980’s, this group began publishing works on both experimental and computational approaches to TKR flexion kinematics and laxity. They first investigated the effect of TKR design on femorotibial contact conditions, experimentally finding the status of the PCL is especially important [85]. Later experimental work focused on the differences between the intact and replaced knee [71], assessing TKR performance during functional activities and constraint using mechanical simulators [86, 87], and most recently investigating the effects of patient and surgical alignment variables [88]. A standard testing method for constraint measurement in TKR (ASTM F-1223 [89]) was based on the approach proposed by Haider and Walker in 2005 [87].

Walker and Garg published a computational study on TKR range of motion using computer graphics models in 1991 [90]. This work predicted maximum flexion of TKR designs, flexion limited by PCL strain limits, finding that the most important surgical variable was sagittal plane tilt of the tibial component. A later study by Sathasivam and Walker predicted TKR kinematics using a computer model with friction, yielding AP displacements and IE rotations comparable to experimental results during laxity and simulated gait tests [91]. Recently, more advanced models
have used rigid body dynamics [92, 93] or finite element [94] analyses to predict joint laxity, and kinematics during more complex motions. In 2008, Moran et al. [95] used a rigid-body-spring contact model to simulate the ASTM TKR laxity standard [89], finding that results were sensitive to secondary motions which are not discussed in the standard. Computational models like this would be able to expedite the design cycle and allow objective comparison between TKR components tested at different locations.

Several published manuscripts have noted the conflicting requirements of laxity and conformity in TKR [8, 72, 73, 96]. In general, lower conformity is necessary for more lax designs, which are generally capable of greater flexion range of motion. Low conformity designs, however, suffer in terms of stability (in extension), wear (due to higher contact stresses), and fatigue damage (due to a highly mobile contact location). High conformity provides very little laxity and reduces the flexion range of motion considerably.

2.8 Design Optimization

Design optimization is a method for determining the best possible design, $\bar{x}$, with respect to one or more performance measures called objective functions, $J(\bar{x})$, while considering any applicable equality, $Ceq(\bar{x})$, and inequality, $C(\bar{x})$, constraints (such as maximum stress or maximum deflection). Design optimization is used heavily in the automotive and aerospace industries, where the demand for optimum strength-to-weight ratios is often a driving factor in design. We seek to reduce the objective function value by manipulating the design vector $\bar{x}$ (a set of parameters describing the design in terms of dimensions and features). An optimum design is one that
cannot be improved any further in terms of the objective function because (a) the best possible performance has been obtained, (b) constraints have shrunk the feasible design space and are limiting the best obtainable performance, or (c) the design space does not include the best design (only the best design within the design space can be found). A typical optimization statement takes the mathematical form:

\[
\begin{align*}
\text{Minimize} & \quad J(\vec{x}) \\
\text{subject to:} & \quad C(\vec{x}) \leq 0 \\
& \quad C_{eq}(\vec{x}) = 0 \\
& \quad \vec{x}_{\text{min}} \leq \vec{x} \leq \vec{x}_{\text{max}}
\end{align*}
\]  

\[ (2.4) \]

2.8.1 Gradient Based Optimization

One of the most widely used design optimization methods is gradient based optimization. In gradient based optimization, a candidate design \( \vec{x}_{\text{candidate}} \) exists somewhere in the allowable design space with a performance of \( J(\vec{x}_{\text{candidate}}) \). The optimizer measures the gradient of the performance with respect to each design variable \( x_i \), normally using a finite differencing method. Using the Steepest Descent Method for gradient based optimizations, the optimizer will following the negative gradient of the performance about the candidate design, \( -\nabla J(\vec{x}_{\text{candidate}}) \) (which is usually calculated using finite differences), and will calculate a new design, \( \vec{x}_{\text{new}} \). The objective function value of \( J(\vec{x}_{\text{new}}) \) should be lower (better) than \( J(\vec{x}_{\text{candidate}}) \). The process flow for a typical gradient based optimization is shown in Figure 2.12. This process iterates
until $J$ ceases to improve and an optimum design is converged upon (Fig. 2.13).

Figure 2.12: Flow chart describing optimization process. An initial design is provided, and the optimizer iterates through designs with increasingly better objective function performance. The optimization completes when the objective function cannot be improved any further and has converged.

2.8.2 Global versus Local Minima

A globally optimum design is one where the objective function cannot be reduced any further within the feasible design space. In optimization, local optima also exist. These are local minima which trap the optimizer, because the local gradient information suggests that any changes to the design will only increase the objective function, but a better design does exist elsewhere in the design space (Fig. 2.14). Local optima pose a challenge in design optimization, because the design space is often a black box (we do not know the exact relationship between our design variables and the objective function). Without completely analyzing the entire design domain, which
is exceedingly difficult and time consuming for any complex design problem, we do not know if we have found a global or local optimum. We can only identify a local optimum if we find a design which outperforms it. We are also unable to reasonably determine how many local optimums might exist. One way to address this problem is to conduct optimization with multiple initial design vectors and select the best optimization result.

2.8.3 Multiobjective Optimization

When one must consider more than one performance measure during optimization, multiobjective optimization (MOO) is used. The simplest approach to multiobjective optimization is to define a new objective function, \( J_{MOO}(w, \bar{x}) \), which is the weighted sum of two objective functions which should both be considered, \( J_1(\bar{x}) \) and \( J_2(\bar{x}) \).
Figure 2.14: Global versus local minimum in gradient based optimization. The optimizer finds the local minimum and stops, even though a better design exists elsewhere in the design space. This can be overcome by using more initial designs to improve the likelihood of ending up at the global minimum.

A weighting factor $w$ is used to specify the relative importance of $J_1(\bar{x})$ and $J_2(\bar{x})$. This is called the weighted sum (WS) approach.

$$J_{MOO}(w, \bar{x}) = w [J_1(\bar{x})] + (1 - w) [J_2(\bar{x})]$$  \hspace{1cm} (2.5)

It is very common in design to have competing objective functions, which is when improvement with respect to one performance measure requires sacrifice in terms of another. Using multiobjective optimization, we can describe this trade-off with a Pareto curve. By varying the weighting function between 0 and 1, we will generate a set of optimum designs, rather than a single optimum. If $J_1(\bar{x})$ and $J_2(\bar{x})$ are competing performance measures, we will find that we get different optimum designs,
depending on the relative importance of the objective functions. Plotting each optimum design on a graph with axis $J_1(\bar{x})$ and $J_2(\bar{x})$, we will define our Pareto or best trade-off curve (Fig. 2.15). The end points of this curve are called the anchor points. These represent the performance of designs optimized for just one objective function, with no consideration of the other. Since the Pareto curve is comprised of optimum designs, no point on the curve outperforms another in terms of both objective functions. The typical Pareto curve shape for competing design variables is shown in Figure 2.16, which is a function of whether $J_1$ and $J_2$ are being minimized or maximized. The value of a Pareto curve is that a designer can easily visualize the relationship between two objective functions. This allows the designer to entertain some preference while knowing how much must be sacrificed in terms of either objective function in order to improve in the other, while still maintaining an optimum design.

2.8.4 Parametric Modelling

Design optimization is usually performed with a computational framework where designs are simulated within different software packages. These simulation packages require part models to represent candidate designs. To perform design optimization, these numerical models must be parameterized. The design vector $\bar{x}$ describes the design, and a modeller uses these instructions to generate a computational model of the part to the exact design specifications. When constructing parametric models of three-dimensional parts, care must be taken to ensure that meaningful designs are generated for any $\bar{x}$ with a high enough model quality that even small design perturbations are reflected by the model. Provided the model accurately depicts these
small perturbations, it is also necessary that the simulations which are performed to evaluate $J(\bar{x})$ provide enough accuracy to be sensitive to small perturbations.

Ideally, parametric models would be robust enough to represent any possible design $\bar{x}$ that the optimizer could request. The number of design variables (or the size of $\bar{x}$), however, greatly influences the number of $J(\bar{x})$ evaluations, and therefore the time required to generate an optimum design. For this reason, the number of design variables must be limited. A combination of intuition, previous experience and resources available all factor in to determining how complex a parametric model can be for a specific optimization problem.
Figure 2.16: The typical Pareto curve shapes that indicate competing relationships for different combinations of objective function maximization or minimization.
2.8.5 Previous Work

The first published TKR optimization was that of Sathasivam and Walker [97]. They used a simplified two-dimensional model of a TKR in the frontal and sagittal planes. The optimization attempted to consider many performance criteria, including contact stress, femoral-tibial size interchangeability, patella lever arm, laxity and stability, and the amount of bone resection required. This work did not use FEA to determine the UHMWPE stresses, instead calculating stresses based on contact patch dimensions from experimental work. A rigorous optimization method, like the gradient based methods described above, was not applied. The resulting approach resembled more of a parameter study than a design optimization. Based on the parameter study results, optimal implant geometry was discussed but it could not be confirmed that a true optimum design had been found. These simplifications are understandable, considering the computational effort required for design optimization and the limited computational resources available in the early 90’s.

Dargahi et al. [98] also attempted optimization of the TKR, but used FEA to calculate UHMWPE stresses. Aside from the use of FEA, their study was similar to that of Sathasivam and Walker [97], although only considering sagittal plane geometry. Wear is assumed to be directly related to contact pressure, while using a realistic wear model which considers contact pressure, sliding distance, sliding direction and contact area would have likely produced different results. Again, a systematic optimization method was not used and the approach was more similar to a parameter study.

Outside of the work described in this thesis, the earliest attempt at three-dimensional shape optimization of a TKR, considering wear rather than contact pressure alone,
was published in 2009 [99]. This work tested the feasibility of using three-dimensional
FE contact analysis and gradient based optimization methods for TKR, although the
TKR geometry was greatly simplified. No authors have published any attempts at
true multiobjective optimization, with multiple performance measures only consid-
ered during parameter studies.
Chapter 3

Wear

3.1 Wear Experiment

Experiments were performed to validate numerical models for wear simulation. The forces applied to the components were validated, as well as the resulting volumetric wear from and damage to the UHMWPE components. Experiment results were first used to tune the wear coefficient $K$ of a novel strain hardening sensitive UHMWPE wear model. $K$ is capitalized to distinguish between this term and the wear coefficient $k$ used in Archard’s classic wear model. The new wear model is described in Sections 3.2 and 3.3. Perturbed loading was used for both experimental and numerical simulations as model validation.
3.1.1 Apparatus

**Force 5\textsuperscript{TM} Simulator Machine**

All wear experiments were performed using an AMTI\textsuperscript{TM} (Advanced Mechanical Technologies, Inc, Watertown, MA) Force 5\textsuperscript{TM} hip / knee simulator (Fig. 3.1). The apparatus consists of servo-hydraulic actuators capable of controlling 4 degrees of freedom when running in knee simulator mode. When configured for TKR wear testing, the degrees of freedom which are fixed, prescribed or unconstrained are described in Table 3.1 and depicted in Figure 3.2. The controller supplies anterior-posterior displacement and flexion-extension of the femoral component using potentiometer feedback. The internal-external rotation of the tibial component is also controlled based on potentiometer feedback, but the axial load is controlled using force feedback from a 6 degree of freedom load cell in the tibial component.

Table 3.1: Status of TKR component DOFs when installed on Force 5\textsuperscript{TM} for wear simulation.

<table>
<thead>
<tr>
<th>Joint DOF</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Medial-lateral</td>
<td>Free</td>
</tr>
<tr>
<td>Anterior-posterior</td>
<td>Prescribed</td>
</tr>
<tr>
<td>Proximal-distal</td>
<td>Prescribed</td>
</tr>
<tr>
<td>Flexion-extension</td>
<td>Prescribed</td>
</tr>
<tr>
<td>Adduction-abduction</td>
<td>Free</td>
</tr>
<tr>
<td>Internal-external</td>
<td>Prescribed</td>
</tr>
</tbody>
</table>

** Samples **

Commercially available implants with matching CAD models were required to allow computational simulations of the experiments. DePuy\textsuperscript{TM} PFC Sigma\textsuperscript{TM} (cruciate
Figure 3.1: AMTI\textsuperscript{TM} Force 5\textsuperscript{TM} hip / knee simulator configured for knee simulator mode. TKR components installed within testing chamber (left) and submerged in bovine serum testing medium.
Figure 3.2: Depiction of AMTI\textsuperscript{TM} Force 5\textsuperscript{TM} configured for knee simulator mode, detailing available degrees of freedom.
retaining, size 3, 8 mm UHMWPE insert) implant components (Figure 3.3) were obtained for wear testing. Multiple UHMWPE inserts were purchased, while only one femoral component and one tibial tray were used for all experiments. This implant provides high conformity in both the frontal and sagittal planes for additional anterior-posterior stability and minimized peak stresses (by maximizing contact area). UHMWPE components are sterilized and stabilized by gamma irradiation in a vacuum foil packaging, which provides a moderate amount of crosslinking. This process addresses oxidative degradation problems which had previously plagued UHMWPE components causing early pitting and delamination [100]. A total of four implants were used for the wear testing experiments, and while a set of samples all from the same batch could not be obtained, production dates were fairly close (Table 3.2). The sample names are based on the production lot names. Two samples were used under identical wear tester loading in order to demonstrate experiment repeatability and to determine a material-specific wear factor. One sample was used for creep and soak control experiments, where only axial loads were applied. One sample was used during experiments with perturbed input load waveforms, in order to validate the tuned wear factor. The intended usage of each sample is shown in Figure 3.4.

Table 3.2: Production lots and dates for UHMWPE components. Sample names are based on production lot names. The intended use for each sample is described briefly under “Purpose”.

<table>
<thead>
<tr>
<th>Implant Name</th>
<th>Production Lot</th>
<th>Production Date</th>
<th>Purpose</th>
</tr>
</thead>
<tbody>
<tr>
<td>J1</td>
<td>BF9GJ4000</td>
<td>Feb. 2007</td>
<td>Wear - original waveforms</td>
</tr>
<tr>
<td>J2</td>
<td>BF9GJ4000</td>
<td>Feb. 2007</td>
<td>Wear - original waveforms</td>
</tr>
<tr>
<td>E</td>
<td>BF9GE4000</td>
<td>Feb. 2007</td>
<td>Creep and soak control</td>
</tr>
<tr>
<td>F</td>
<td>BC4F84000</td>
<td>Jan. 2007</td>
<td>Wear - perturbed waveforms</td>
</tr>
</tbody>
</table>
CHAPTER 3. WEAR

Figure 3.3: DePuy™ PFC Sigma™ CR implant used for wear experiments. The femoral component and tibial tray were reused, but new UHMWPE inserts were installed for each experiment.

Figure 3.4: The intended usages of each UHMWPE component during experiments. Implants J1 and J2 are used for testing experiment repeatability, simulation tuning and validation. Implant E is used for soak control experiments. Implant F was used for simulation validation only.
Tray Lock Modification

The UHMWPE component snap-fits into place on the tibial tray via a locking mechanism on the anterior edges of the components. The locking mechanism is designed to hold the component securely and reduce backside motion (relative displacement between the UHMWPE component and tibial tray) as much as possible. The consequence is that removing the UHMWPE component will normally cause some permanent damage to the locking mechanism, reducing fixation strength if the same UHMWPE component is reinstalled, and possible fracturing. Since wear measurements were to be made every 500,000 wear cycles using a gravimetric method, the locking mechanism had to be revised to allow easy removal and reinstallation without compromising fixation strength or removing any material (which could not be measured and would compromise the gravimetric measurements). The anterior edge of the tibial tray was removed by a simple milling operation, and acrylonitrile butadiene styrene (ABS plastic) clamps were printed on a three-dimensional printing machine (Fig. 3.5). The revised locking system provided adequate fixation, but simply loosening a bolt holding the ABS plastic clamp in place released the anterior edge of the UHMWPE component, allowing safe removal. A similar approach has been used by other authors [101], although in that case the clamp was machined from steel, not printed from ABS plastic.

Component installation

The DePuy™ femoral component was attached to a plastic mounting jig using bone cement, and the plastic mounting jig attached to the Force 5™ femoral component shaft with a single machine screw. The tibial tray was cemented into the Force
Figure 3.5: The clamp designed to replace the anterior edge locking mechanism of the tibial tray. The clamp was printed from ABS plastic and held in place by a bolt.

5™ tibial component, which was then placed on top of the tibial load cell with all relative degrees of freedom fixed except the adduction-abduction rotation and medial-lateral displacement (Fig. 3.6). While the ISO standard for wear testing suggests that components be aligned such that the axial load is offset medially to increase medial condyle loading, no offset was used in these experiments. Since experiments were only for comparison with our own simulations which had matching conditions, this positioning was acceptable.

Figure 3.6: The ML displacement and AA rotation joint at the tibial load cell. ML displacement and AA rotation are provided by a combined sliding / pivoting joint between the tibial load cell and tibial component (middle). The assembled configuration is shown on the right.
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Testing Environment

To make experiment results as relevant as possible, the testing enclosure for the samples was a controlled environment. An IV bag enclosed the testing volume including the femoral component and UHMWPE insert (Fig. 3.1). A 50% bovine serum solution was used as the testing medium, and was circulated from a heated external bath and into the testing environment using a peristaltic pump. The testing medium drained out of the testing environment, back into the bath. The bath temperature was controlled by a built-in thermostat, while the temperature of the fluid within the testing environment was monitored using a thermocouple. The bath temperature was regulated such that the temperature within the testing environment remained close to 37°C. The 50% bovine serum solution was prepared and replaced during wear measurements every 500,000 cycles. The fluid consisted of:

- deionized water, 0.5 L per 1 L final solution
- ethylenediaminetetraacetic acid (EDTA), 5.8 g per 1 L final solution
- amphotericin-B (Fungizone), 10 mL per 1 L final solution
- adult donor bovine serum (∼70 g/L total protein content), 0.5 L per 1 L final solution

EDTA binds to calcium in solution to avoid calcium phosphate precipitation onto the UHMWPE bearing surface [102]. To minimize microbial contamination, fluids remained frozen until they were required for testing, and amphotericin-B was included in the final mixture. The final protein concentration of the fluid (∼35 g/L) was well above the minimum of 17 g/L specified in ISO the standard [40].
3.1.2 Loading

The apparatus used displacement control for the anterior-posterior displacement, flexion-extension and internal-external rotation degrees of freedom. While standard displacement controlled waveforms exist, the kinematics are prescribed and are insensitive to the shape of the implant components. Actual knee kinematics are a function of the forces applied, contact geometry and soft tissue contributions, so force-controlled standards are preferred. The force control standard for TKR wear testing, ISO 14243-1 [40] prescribes forces at the knee which are similar to the conditions seen during gait, and springs resisting AP translation (30 N/mm) and IE rotation (0.6 Nm/deg) should be used to simulate soft tissue contributions. In order to obtain appropriate implant kinematics for the particular TKR design, while working within the constraints of our displacement controlled machine, the following 3 steps were taken:

1. A quasi-static finite element contact analysis with 80 load steps was performed in order to simulate a single wear test cycle using ISO 14243-1 [40] loading. Soft tissue springs were included in the FE model in accordance with the ISO standard, but the axial load through the UHMWPE insert was not offset medially. This simulation calculated what the resulting kinematics would be if the Force 5™ machine were force controlled.

2. The resulting displacements were used as inputs for the displacement controlled machine. The machine was tuned to match these input displacements as closely as possible, but was limited by stability and dynamic factors. The resulting loads / displacements were measured and recorded.
3. The resulting loads / displacements were used as inputs for the displacement controlled simulation. Resultant force and moment data from the simulation were compared to loads measured during the experiment in order to judge how well the actual mechanics of the wear tester are simulated \textit{in-silico}.

For more details on the FE model, which was subsequently used for wear simulations, refer to 3.3.1.

The anterior-posterior and axial forces, internal-external torques and flexion-extension were taken directly from the ISO standard (aside from the internal-external torques being inverted) and appropriate AP displacement and IE rotations were calculated in the manner described above. For meaningful validation with the experimental results, perturbed conditions also had to be considered. A second set of waveforms were therefore generated, which used the ISO standard forces with the exception that the internal-external torques were doubled, and appropriate displacements were calculated. The resulting displacements for the original and perturbed experiment conditions are shown in Figure 3.7. It should be noted that the AP displacements and IE rotations are represented in terms of relative motion of the tibial component with respect to a global coordinate system. The original waveforms were used for two experiments, using samples J1 and J2. A third experiment used sample E under only axial loading in order to study mass increases due to protein / moisture uptake (loaded soak control) and creep. The fourth experiment used the perturbed waveforms, for wear testing of sample F (Table 3.2).
Figure 3.7: Force 5™ input waveforms for original (solid) and perturbed (dashed) experiments. Original waveforms are based on ISO standard loading. Perturbed loadings featured increased IE rotations due to doubling the IE torques.
3.1.3 Experiment Protocol

Gravimetric Measurements

Before any mass measurements were made using the analytical balance (Fisher-Scientific™ AccuSeries™ 225D, 0.01 mg resolution), clean and dry samples were placed beside the balance for 30 minutes to acclimatize to the room temperature and humidity. From this point forward, the samples were only handled with Kelly forceps as it was found that any touching, even when wearing nitrile gloves, caused relatively large fluctuations in mass. Each sample was measured a minimum of 3 times, as well as a 20 g calibration mass used to account for balance drift. Each sample average mass was corrected by the average calibration mass change.

Pre-soaking

UHMWPE components submerged in a bovine serum solution will increase in mass due to moisture and protein absorption [41, 103, 104]. In order to account for this, wear experiments are normally accompanied by a loaded soak control specimen. This UHMWPE component undergoes the same axial loading through contact with a femoral component while immersed in a bovine serum solution. No other loads or displacements are applied, however, so relative motion between the components are minimal, and wear of the UHMWPE component is negligible. This allows researchers to measure and account for the change in mass due to moisture / protein uptake in the actual testing specimens.

All UHMWPE components were initially immersed in a bovine serum bath at 37°C for a minimum of 3 weeks without load. During this phase, mass increase was rapid and nonlinear, but by the end reached a nearly constant rate. A soak
control function (Fig. 3.8) was derived based on the mass increase of a sample over time while unloaded. During an axially loaded soak control experiment, the mass change after correction using the unloaded soak control function was negligible. This suggested that loaded and unloaded mass increase rates were sufficiently similar and the unloaded soak control function was adequate for correction of loaded sample data.

Figure 3.8: Soak control curve for correcting sample mass measurements. Negligible differences between loaded and unloaded uptake rates suggested that unloaded soak control data was sufficient.

Sample Testing

After a sample pre-soaking period was complete, it was ready for wear testing in the Force 5\textsuperscript{TM}. The UHMWPE insert sample was installed onto the tibial tray using the modified locking mechanism described in 3.1.1. A 2000 mL IV bag enclosed the testing
environment and with the Force 5\textsuperscript{TM} running in low-pressure mode (approximately 100 psi), axial load was increased until the femoral component and UHMWPE insert came into contact. With the contact closed, the Force 5\textsuperscript{TM} was switched into high-pressure mode (approximately 750 psi), which allowed the machine to match input force / displacement waveforms with minimal error. The fluid handling system was activated to circulate the bovine serum solution through the testing environment, and the wear test was started using the desired input waveforms. The cycle rate was set to 1 Hz, close to the rate of natural gait, and 500,000 cycles were allowed to pass before the machine was stopped. A graceful finish at 500,000 test cycles froze all of the actuators at their correct position in the cycle and held them fixed until some user intervention.

Several experiments were interrupted prematurely for reasons related to power failures, testing fluid leakage, or over-heating related to Force 5\textsuperscript{TM} or chiller malfunctions. Depending on the severity of the interruption, the machine was simply restarted, the fluid was replaced, or the components were removed and placed in a bovine serum bath while major repairs took place. The longest such interruption was nearly 4 months, during which time a complete overhaul of the Force 5\textsuperscript{TM} motor and hydraulic pump was necessary. The wear rates before and after the delay, however, were still in good agreement.

After 500,000 cycles, the UHMWPE components were removed from the apparatus and underwent a stringent cleaning and drying regime. This is outlined in appendix A.

Following cleaning, the samples were measured as described earlier in Gravimetric Measurements. Once gravimetric measurements were made, the contact
surfaces of the UHMWPE samples were measured using a ShapeGrabber™ (Shape-Grabber, Ottawa, Ont.) SG series laser scanner (Fig. 3.9). The sample was laid flat and 8 scans were made, rotating the sample 45° for each scan. The sample was then tilted to an angle of 30° to the horizontal, towards the scan head, and 8 more scans were made. This scanning procedure ensured that reliable scan data for the entire contact surface was obtained. If any areas of particularly bad scan quality were identified, further scanner passes were performed. The scan data produced three-dimensional surfaces on a 0.05 mm x 0.05 mm grid. The actual accuracy of the scan data, however, was not verified for UHMWPE components and was intended to provide (at most) a qualitative measure of the damage distribution.

Figure 3.9: Depiction of the laser scanner system used to measure contact surface topography. A laser beam emitted above the sample reflects off the contact surface and is measured by the scan head. The scanner passes over the surface sampling data every 0.05 mm. The orientation of the sample is changed after each scanner pass.

Before reinstalling the UHMWPE sample, the testing environment was cleaned and disinfected with a 10% bleach solution and rinsed thoroughly with deionized water. A new batch of 50% bovine serum solution was prepared as described in 3.1.1, components were reinstalled, and the next 500,000 cycles of wear testing were
initiated. This entire process iterated seven times until a total of 3.5 million cycles were completed.

3.1.4 Data Management

Load cell and displacement data was captured at multiple intervals throughout the experiments, at least twice during each 500,000 cycle testing period. Each recording contained several cycles worth of data, including the forces and torques measured by the 6 DOF load cell, and various potentiometer readings including flexion-extension, anterior-posterior displacement and internal-external rotation.

Random temperature checks were made periodically throughout the experiments (at least twice during each 500,000 cycle testing period) to ensure that the temperature within the fluid environment was approximately 37°C as measured by the thermocouple. If necessary, adjustments were made to the fluid bath temperature thermostat.

The laser scan data required further processing after the scans were gathered. The individual scans were manually inspected, and voids in the surface data were normally present, due to reflection issues from the concave UHMWPE surface. The data points surrounding these voids were assumed to be unreliable, so perimeter data was trimmed. This was done automatically using the scanner software which could identify and remove any perimeter data (from around voids, and around the outer periphery of the entire scan). Since approximately twenty scans of the surface were obtained, the data missing from the void could always be provided by one of the other scanner passes. Once trimming was complete, scans were manually aligned, then auto-aligned using a least-squares best fit alignment program within the scanner.
software. Once aligned, the software was able to combine the multiple scans from a single measurement set into a single surface (3.10).

![Figure 3.10: Voids are present in the data from a single scan (left). Data surrounding the voids is assumed unreliable and also removed from the data set (middle). Multiple surface scans from the same measurement set are combined in order to create a single surface with no voids (right).]

In order to visualize the damage distribution across the contact surface of an implant, the combined surface from one measurement set could be compared to the combined surface from an initial (reference) measurement set. Surfaces were aligned by a least-squares best fit comparison, only considering areas of the surface which were known to have not undergone wearing. Once aligned, the damage depth distribution was represented by the gap between the original and worn surfaces.

As well as laser scanning, the damage patch was inspected visually. The outer periphery of the damage patch was marked with a fine tipped marker, and the contact surface was optically scanned with a desktop scanner.

The same data collection procedure was repeated during the experiments with all four samples.
3.2 Frictional Work based Wear Model

The classic wear model first described by Archard and Hirst [42] is insufficient for characterizing ultra high molecular weight polyethylene (UHMWPE) wear because it does not account for strain hardening. A new wear model had to be developed which could predict UHMWPE wear under different kinematic conditions with a consistent wear factor $K$.

A unique strain hardening sensitive UHMWPE wear model was developed, and is a significant contribution in this thesis. The proposed strain hardening UHMWPE wear model is based on the assumption that wear at the surface of these polymers can be approximated by the wear of two separate polymer fractions (Fig. 3.11). The first fraction is composed of polymer molecules whose orientations are completely multi-directional. In this fraction, there is no predominant molecular orientation (PMO), and we also assume this is the initial state of new UHMWPE. The second fraction is composed of polymer molecules completely aligned with a PMO, which we assume is a completely strain hardened fraction of UHMWPE. We assume that a single point on the surface of the UHMWPE component is composed of the sum of these two fractions, and we define the composition by the percentage which is aligned, $\beta$ ($0 \leq \beta \leq 1$). The total wear depth at any point will be the weighted sum of the wear from the multidirectional fraction $\delta_{multi}$ and the aligned fraction $\delta_{aligned}$, such that:

$$\delta_{wear} = \beta \delta_{aligned} + (1 - \beta) \delta_{multi} \quad (3.1)$$

It should be noted that $\beta$ and $\delta_{aligned}$ are functions of the amount and direction of frictional work with respect to the PMO, $\theta$. $\delta_{multi}$ is a function of the total amount
of frictional work, and is insensitive to $\bar{\theta}$. This method relies heavily on the principle of frictional work, which was used in a theoretical UHMWPE wear model introduced by Wang [28]. The approach used to calculate $\beta$ and the implementation of the two-phase assumption are novel to this model.

![Illustration](image)

Figure 3.11: Illustration depicting of multidirectional versus unidirectional (aligned) polymer fractions. The natural and unworn surface of UHMWPE is assumed to be composed of randomly oriented molecules. Due to strain hardening, the molecules align with a predominant orientation.

### 3.2.1 Step 1 - Calculating $\beta$

We must calculate the fraction of aligned molecules. The reorientation of the polymer molecules is induced by counterface sliding in a predominant direction. We assume that the PMO ($\bar{\theta}$) will align with the direction of maximum frictional work expenditure, or the direction perpendicular to that of minimum frictional work. As previously described by Wang in 2001 [28], the amount of frictional work expended along $\bar{\theta}$ during a given duration divided into $n$ increments can be expressed as:

$$W_{\parallel} = \sum_{i=1}^{n} (|q_i| |s_i| \cos^2 (\theta_i - \bar{\theta})) = \sum_{i=1}^{n} (\mu P_i |s_i| \cos^2 (\theta_i - \bar{\theta}))$$  \hspace{1cm} (3.2)
where $\mathbf{q}_i$ is the tangential (frictional) force vector (parallel to the surface) resisting sliding and $\mathbf{s}_i$ is the sliding distance vector (along the surface). $P_i$ is the normal force acting on the surface due to contact and $\mu$ is the coefficient of friction. $\theta_i$ is the current sliding direction. The amount of frictional work expended perpendicular to $\bar{\theta}$ can be expressed as:

$$W_{\perp} = \sum_{i=1}^{n} (|\mathbf{q}_i||\mathbf{s}_i|\sin^2(\theta_i - \bar{\theta})) = \sum_{i=1}^{n} (\mu P_i |\mathbf{s}_i| \sin^2(\theta_i - \bar{\theta})) \quad (3.3)$$

The total frictional work is simply:

$$W_{\text{tot}} = \sum_{i=1}^{n} (|\mathbf{q}_i||\mathbf{s}_i|) = \sum_{i=1}^{n} (\mu P_i |\mathbf{s}_i|) \quad (3.4)$$

In order to find $\bar{\theta}$, we perform an optimization problem (at each point on the contact surface, as each point may have a different $\bar{\theta}$) in order to minimize $W_{\perp}$ (or maximize $W_{\parallel}$), expressed mathematically:

Minimize $W_{\perp}(\bar{\theta})$

where: $W_{\perp}(\bar{\theta}) = \sum_{i=1}^{n} (\mu P_i |\mathbf{s}_i| \sin^2(\theta_i - \bar{\theta})) \quad (3.5)$

$i = 1, ..., n$ (number of substeps)

An exhaustive search method for $\bar{\theta}$ should be used for the minimization problem, in order to avoid the possibility of finding only a local minimum. This involves calculating $W_{\perp}$ at 1800 increments between $\bar{\theta} = 0$ and $\bar{\theta} = \pi$ and selecting the $\bar{\theta}$
which minimizes $W_\perp$.

With $\bar{\theta}$ now known, we need to calculate the amount of crossing motion $\sigma$ ($0 \leq \sigma \leq 1$), also known as the crossing intensity. Similar to the approach of Kang et al. [23, 62, 105], we define $\sigma$ as twice the ratio of perpendicular work $W_\perp$ to total work $W_{tot}$ (doubled to normalize between 0 and 1, as the maximum possible ratio of perpendicular work to total work is 0.5):

$$\sigma = \frac{2W_\perp}{W_{tot}} = \frac{2 \sum_{i=1}^{n} (\mu P_i |s_i| \sin^2 (\theta_i - \bar{\theta}))}{\sum_{i=1}^{n} (\mu P_i |s_i|)} = \frac{2 \sum_{i=1}^{n} (P_i |s_i| \sin^2 (\theta_i - \bar{\theta}))}{\sum_{i=1}^{n} (P_i |s_i|)}$$

which is also minimized by the correct selection of $\bar{\theta}$. $\sigma$ will be a value between 0 and 1; 0 for completely unidirectional counterface motion and 1 for completely multidirectional counterface motion. It should be noted that in the works of Kang et al. [23, 62, 105], $\sigma$ is denoted $CS$ (cross shear) and is not normalized to 1, so $0 \leq CS \leq 0.5$.

We calculate the amount of alignment by assuming that $\beta = 1 - \sigma$, or:

$$\beta = \frac{W_{tot} - 2W_\perp}{W_{tot}} = \frac{\sum_{i=1}^{n} (P_i |s_i|) - 2 \sum_{i=1}^{n} (P_i |s_i| \sin^2 (\theta_i - \bar{\theta}))}{\sum_{i=1}^{n} (P_i |s_i|)}$$

### 3.2.2 Step 2 - Calculating $\delta_{\text{multi}}$

$\delta_{\text{multi}}$ is the damage of the completely multidirectionally aligned polymer fraction. Without any predominant orientation in these molecules, we can assume that we
have equal frictional work expenditure both along and perpendicular to the molecules. We assume that only frictional work perpendicular to the molecules will contribute to wear, while frictional work along the molecules contributes to further strain hardening (further molecular alignment) [28]. This means that the amount of frictional work contributing to wear is $\frac{1}{2} W_{\text{tot}}$. We introduce the material specific wear parameter, $K$, which is unique to the specific UHMWPE being used. The amount of material removed due to contributing frictional work will be proportional to $K$, such that:

$$\delta_{\text{multi}} = \frac{1}{2} K W_{\text{tot}} = \frac{1}{2} K \sum_{i=1}^{n} (\mu P_i |s_i|) = \frac{1}{2} K \mu \sum_{i=1}^{n} (P_i |s_i|)$$ (3.8)

### 3.2.3 Step 3 - Calculating $\delta_{\text{aligned}}$

In the completely strain hardened or aligned fraction of UHMWPE, we again assume that only frictional work perpendicular to the molecules will contribute to wear. In this fraction, we have assumed that all molecules are aligned with a PMO, $\bar{\theta}$, so the wear can be calculated using:

$$\delta_{\text{aligned}} = K W_\perp = K \sum_{i=1}^{n} (\mu P_i |s_i| \sin^2 (\theta_i - \bar{\theta})) = K \mu \sum_{i=1}^{n} (P_i |s_i| \sin^2 (\theta_i - \bar{\theta}))$$ (3.9)

### 3.2.4 Step 4 - Calculating $\delta_{\text{wear}}$

The total wear damage is calculated by substituting Equations 3.7, 3.8 and 3.9 into Equation 3.1:
CHAPTER 3. WEAR

\[
\delta_{wear} = \beta \delta_{aligned} + (1 - \beta) \delta_{multi}
\]
\[
= K \mu \left[ \beta \sum_{i=1}^{n} (P_i |s_i| \sin^2 (\theta_i - \bar{\theta})) + (1 - \beta) \frac{1}{2} \sum_{i=1}^{n} (P_i |s_i|) \right]
\]

where

\[
\beta = \frac{\sum_{i=1}^{n} (P_i |s_i|) - 2 \sum_{i=1}^{n} (P_i |s_i| \sin^2 (\theta_i - \bar{\theta}))}{\sum_{i=1}^{n} (P_i |s_i|)}
\]

\[i = 1, ..., n \text{ (number of substeps)}\]

We can use this approach to find the total damage for \(n\) substeps at any point on the contact surface of an UHMWPE component. When used with a discretized area as in finite element analysis, we can calculate our volumetric wear over a finite area based on the damage depths at each corner node of that area. The volumetric wear from a single finite element can be approximated as the area of that element, multiplied by the average nodal damage depth.
### 3.2.5 Similar Wear Model

At this time, the closest comparable model to the one described above is the work of Kang [62]. The model takes the form:

\[
\delta = K(CS) \sum_{i=1}^{n} P_i |s_i| \\
i = 1, ..., n \text{ (number of substeps)}
\]

\[
CS = \frac{W_\perp}{W_{\text{tot}}} \tag{3.11}
\]

where the relationship between \(CS\) and \(K\) is determined by fitting different models to experimental pin-on-disk experiment measurements using power function, piece-wise linear regression and logarithmic expressions. The model has been developed based on the unified theory of wear and frictional work proposed by Wang [28], however takes a different form than our proposed model. This form requires more experiment parameters to define the relationship between \(CS\) and \(K\), while our method assumes that the \(K\) parameter is material-specific and is independent of the amount of crossing motion. Another significant difference between these two models is the assumption of two polymer fractions in our model. In Kang’s model, the basic assumption is that wear is only caused by frictional work perpendicular to the predominant molecular orientation. In our model, this is indeed how wear is generated from the fully aligned fraction, whereas there is also a multidirectional polymer fraction where half of the total frictional work will contribute to wear. In reality, the surface composition would be a gradient between molecules completely aligned with a PMO and molecules randomly oriented. Figure 3.12 depicts the effective wear factor across the total range.
of possible amounts of crossing motion, normalized with respect to the effective wear factor for zero crossing motion \((K_{\text{unidirectional}}, 0)\) and completely multidirectional motion \((K_{\text{multidirectional}})\) for both models. It is interesting to note that for the extreme cases of fully unidirectional motion and fully multidirectional motion, these models actually yield the same results. It is for motions between these two extremes where we see differences in the two models.

Figure 3.12: A plot of the effective wear factor versus cross shear ratio for the newly developed wear model and the model described by Kang [62]. At the extreme conditions of minimum or maximum CS, the models predict the same effective wear factor.

### 3.3 Wear Simulation

Wear simulations were performed in order to compare with the wear experiments and test the validity of the UHMWPE wear model proposed in 3.2.
3.3.1 FE Model

Finite element meshes of the implant components were created from available CAD models of the femoral component and UHMWPE insert of a size 3 DePuy™ PFC Sigma™ CR implant using HyperMesh™ (Altair Engineering Inc, Troy, MI). The CAD models contained a lot of information on the non-contacting surface geometry of the components, such as the bone-implant interface of the femoral component and the locking mechanism of the UHMWPE insert. These features were not required for wear simulations, as they have no impact on the nature of the contact conditions. The implant components were defeatured such that only the pertinent contact geometry and underlying shape were maintained. The UHMWPE CAD model was for a thicker than 8 mm component, but the thickness was easily cropped to the appropriate size, since the contact geometry was identical.

The UHMWPE component was meshed with $\sim$4500 8-noded linear hexahedral volume elements, created by first meshing the contact surface with $\sim$900 quad elements and then sweeping that mesh through the solid. The resulting mesh had 5 layers of elements, with an average edge length of 2 mm (Fig. 3.13).

Compared to the UHMWPE component, the femoral component is several orders of magnitude stiffer and could be considered a rigid surface. The contact surface was meshed with $\sim$2500 second-order tria-shaped elements (Fig. 3.14). A mesh convergence study was performed with a similar (but parametric) FE model and it was determined that a mesh with element edge lengths averaging around 2 mm used for both components was adequate for calculating wear.
Figure 3.13: Linear hexahedral FE mesh of UHMWPE insert used during wear simulations. The average element edge length of 2 mm resulted in 5 layers of elements; approximately 4500 elements in total.

Figure 3.14: Second-order rigid tria FE mesh of the femoral component contact surface used during wear simulations. Approximately 2500 elements were used for the surface. The surface was modelled as a rigid body due to the stiffness of the femoral component with respect to the relatively soft UHMWPE insert.
Material Properties

The UHMWPE was modelled as a nonlinear elastic isotropic material derived from the modulus–stress data by Cripton [106] (Fig. 3.15). The data corresponds to UHMWPE at 37°C, and beyond stresses of 17 MPa, the stress-strain relationship changes to purely linear [107]. The Poisson’s ratio was 0.44.

![Graph](image)

Figure 3.15: Modulus–stress data for UHMWPE at 37°C (left) was used to derive nonlinear elastic isotropic stiffness curve (right) for the UHMWPE insert component FE model. A bilinear assumption for the modulus–stress data simplified the material model.

The femoral component was modelled as a rigid surface, so no material properties were defined.

Contact Properties

Contact between the femoral component and UHMWPE insert contact surfaces was modelled using the ANSYS\textsuperscript{TM} V11 (ANSYS Inc., Canonsburg, PA) surface-to-surface TARGE170 and CONTA173 contact elements, respectively. The Augmented Lagrange method was used (see 2.1), with a maximum allowable penetration depth of 0.1 mm and an initial contact stiffness scaling factor of 0.5. Using this approach, the contact stiffness is automatically adjusted to ensure no penetration depths exceed the criterion. The coefficient of friction between the two components was assumed to be
Pilot Nodes and Multi-Point Constraint Joints

Pilot nodes are individual 6 degree of freedom nodes which are capable of relaying forces and displacements to larger meshed components. Pilot nodes were used to guide both the femoral component and UHMWPE insert. The femoral component pilot node was positioned as to provide the same flexion-extension axis for the FE model as in the experimental apparatus. The UHMWPE insert pilot node was positioned with respect to the UHMWPE in such a manner as to provide the same tibial kinematic conditions as the experimental apparatus. Multi-point constraint (MPC) joints were used in order to provide the same tibial degrees of freedom, requiring a cylindrical joint (providing axial displacement and internal-external rotation), a revolute joint (providing adduction-abduction) and a prism (slider) joint (proving medial-lateral displacement). The configuration of these joints is outlined in figure 3.16. The degrees of freedom at the pilot nodes were constrained to match those of the experimental apparatus, constraining all but the flexion-extension and anterior-posterior displacement degrees of freedom for the femoral component. The UHMWPE insert pilot node, along with the MPC joints, accommodated axial displacement, medial-lateral displacement, adduction-abduction and internal-external rotation (Fig. 3.17).

Simulated Springs

AP and IE restraint was provided by spring elements. A spring element on the femoral pilot node with a stiffness of 30 N/mm resisted AP translations. A rotational spring element was placed parallel to the cylindrical MPC joint of the tibial component with a
Figure 3.16: Force 5™ tibial component degrees of freedom simulated using MPC joints in ANSYS™. A cylindrical joint provided IE rotation and axial displacement / load. A revolute joint allowed AA rotations, and a prism joint allowed ML displacements.
Figure 3.17: Femoral and tibial degrees of freedom provided during FE simulations in ANSYS™. Loads and displacements were transferred to implant components through pilot nodes.
stiffness 0.6 Nm/deg to resist IE rotations. These springs are part of the ISO standard wear testing configuration [40], which also prescribes the spring stiffnesses. During force controlled simulations, these springs would resist displacements, but served no purpose during displacement controlled simulations and were then removed.

3.3.2 FE Simulation

The finite element model described above was imported into ANSYS™ V11 for quasi-static contact analysis. The first step of the simulation displaced the tibial component vertically to come into contact with the femoral component. Contact closure can pose convergence problems, especially when contact is driven by applied forces, so this step helped to reduce simulation time. With the contact closed, the displacement condition was replaced with an axial force equal to the axial load at the beginning of the ISO wear testing standard, and the contact problem was again allowed to converge. The force / displacement waveforms being simulated were broken down into a series of 80 load steps. The simulation progressed through each step, resolving the converged contact conditions including contact pressure and sliding distances during each load step. The ANSYS™ nonlinear geometry option was active, which increased computation time but was necessary due to large rotations present in the simulation. Each loadstep required at least 2 iterations for the contact problem to converge, with a maximum of 27 iterations per loadstep. If the contact problem had not converged by the end of a loadstep, or predictors determined that convergence was unlikely, the loadstep would be bisected into smaller substeps and more attempts were made.
3.3.3 Post-Processing

After all loadsteps were simulated, the ANSYS™ post-processor looped through the results data and exported:

- the contact pressure at each integration point, of each UHMWPE contact element, at each loadstep
- the sliding distance in orthogonal coordinates at each integration point, of each UHMWPE contact element, at each loadstep
- the area of each UHMWPE contact element
- the maximum von-Mises stress at any UHMWPE hexahedral element at any loadstep

Calculating Creep Damage

Further post-processing was performed in Matlab™ (The MathWorks, Natick, MA), which read in the results data from the files. Stepping through the load step results, the code first calculated the amount of creep damage caused during the desired number of simulation cycles. The average contact pressure at each node was determined. The corresponding amount of nodal creep damage was then estimated using Equation 2.2, which calculates creep based on the average contact pressure, average UHMWPE insert thickness at the contact surface, the amount of previous creep damage and the duration of loading.

It was important that the amount of previous creep damage be considered, as this model assumed that creep damage was permanent and only progressed when sufficient load was present. This is shown using a displacement history in Figure 3.18. At $t_1$, ...
an initial load of $p = 10$ MPa was applied, until $t_2$ when the load was increased to $p = 20$ MPa, then reduced to $p = 5$ MPa at $t_3$. From $t_1$ to $t_2$, the creep damage curve follows the curve for $p = 10$ MPa. When the pressure is increased, the creep damage follows the curve for $p = 20$ MPa, but for continuity must start from a point on that curve such that $\text{Creep}(20, t) = \text{Creep}(10, t_2)$. This curve is followed until $t_3$, at which point the curve must follow the curve for $p = 5$. Since the $p = 5$ curve appears to level off far below the current creep damage of approximately 0.55 mm at $t_3$, no further creep damage occurs from $t_3$ to $t_4$.

Figure 3.18: Model for estimating creep progression at a single point on the UHMWPE contact surface. The applied load ($p(t)$) changes at $t_2$ and $t_3$. The resulting creep damage is a function of the applied load, the duration the load has been applied, and the previous damage before the load was modified. Creep damage is permanent and only progresses when sufficient load is applied.

A condition was built into the post-processor to ensure that the maximum incremental creep damage at any node would not exceed 0.1 mm. If the creep damage
criterion was violated, the number of cycles currently being simulated was decreased until the criterion was satisfied. This meant extra simulation iterations, especially early in the cycle count when creep progressed most rapidly.

Calculating Wear Damage

At each integration point, the predominant polymer orientation \( \bar{\theta} \), the fraction of aligned UHMWPE \( \beta \), and the total wear damage \( \delta_{\text{wear}} \) were calculated using the integration point sliding distances (in orthogonal directions) and contact pressure with Equation 3.1. The damage depth was scaled by the number of cycles being considered. Wear damage was first calculated at each integration point, used to calculate the element-wise volumetric wear based on the average wear depth across the element and the element area. The nodal wear damage was then calculated by averaging surrounding integration point data.

The total damage depth at a node was the sum of the incremental wear and creep damage. Another condition was built into the code to ensure that the maximum incremental damage (wear + creep) was less than 0.15 mm. Once again, if the condition was violated, the number of cycles considered was reduced.

Nodal Updating

The long term effects of the combined wear and creep damage on the surface of the implant was simulated by actually perturbing surface nodes. Once the total damage depth at each node was known, the node was perturbed normal to the contact surface. The result was a worn patch on the contact surface, but large damage depths risked reducing the mesh quality in the layer directly below the contact surface. To account
for this, a mesh smoothing operation performed during each iteration distributed the perturbation throughout the mesh (Fig. 3.19). This ensured a good quality mesh even with large damage depths.

Figure 3.19: Mesh smoothing was performed in HyperMesh™ to prevent mesh distortion. Once the surface nodes are perturbed, the underlying mesh is adjusted to distribute the distortion throughout the entire mesh.

**Iteration and Data Collection**

The process described above was repeated for all desired cycle intervals. For comparison with experiments, simulation results were calculated at every 500,000 cycle interval, up to 3.5 million cycles. If the creep or total damage criterion were violated, additional simulations were performed. Typically, iterations with a smaller number of cycles were required at the beginning of the wear simulation due to the nonlinear progression of creep damage. Once the creep rates stabilized, the 500,000 cycle iterations were sufficient (in terms of the creep and total damage criterion) and no further iteration bisections were necessary. The framework for this simulation is depicted in Figure 3.20.

The resulting data from the wear simulation included the cumulative volumetric wear at each interval, the cumulative damage distributions (wear, creep, and total), as well as the forces through the tibial component. Other simulation results such as maximum von-Mises stress, crossing ratios and tribological intensities were also saved,
Figure 3.20: Flow chart depicting computational framework to simulate wear. Conditions on maximum creep and total damage depths may require more iterations than those requested by the user.
but a means of measuring these values experimentally was not readily available.

3.4 Wear Experiment versus Simulation

The wear model required tuning for the wear coefficient $K$. Once the $K$ value was tuned, extra steps were taken to ensure that $K$ was still valid under perturbed conditions. The tuning and validation results are discussed here.

3.4.1 Results

Tuning Wear Model using Original Loading

The objective of the tuning procedure was to find a value for $K$ such that experiments using a given implant and loading conditions could be simulated with the numerical model with matching results. Gravimetric wear measurements were made during 2 experiments using the original loading condition. After correcting for fluid uptake using the soak control function and assuming a density of 0.94 mg/mm$^3$ for UHMWPE, the mean volumetric wear after 3.5 million cycles was found to be 26.9 mm$^3$ (25.3 mg). The material specific wear parameter $K$ was tuned such that the simulation predicted the same total volumetric wear under the original loading condition (26.6 mm$^3$), requiring $K = 1.0\times 10^{-6}$ mm$^3$/Nmm. The predicted damage distribution at 3.5 million cycles was compared to the experimentally observed surface damage (Fig. 3.21).
Figure 3.21: Experimentally observed (left), simulated (middle) and outlined experimental versus simulated damage patches (right) under original loading condition. Simulated damage contours and iso-lines are in 0.05 mm increments. Good agreement between the simulated and experimentally derived damage patches is indicated by similar perimeter shapes in the right image (simulated=solid, experiment=dots).
Wear Model Validation using Perturbed Loading

A wear simulation was performed using the tuned model with perturbed loading conditions for validation. The calculated wear after 3.5 million cycles was 48.6 mm\(^3\), compared to 49.0 mm\(^3\) (46.0 mg) measured experimentally (0.8% difference). The simulated damage distribution after 3.5 million cycles compared to the experimentally measured damage distribution is shown in Figure 3.22. Figure 3.23 plots all of the simulated and observed wear measurements for all loading conditions.

![Image of damage distribution](image)

Table 1 summarizes the normalized root mean square (nRMS) prediction errors. nRMS values are the error divided by the total range of that data.

<table>
<thead>
<tr>
<th></th>
<th>Medial Maximum</th>
<th>Lateral Maximum</th>
<th>Medial Maximum</th>
<th>Lateral Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>nRMS</td>
<td>0.360 mm</td>
<td>0.347 mm</td>
<td>0.264 mm</td>
<td>0.265 mm</td>
</tr>
</tbody>
</table>

Figure 3.22: Experimentally observed (left), simulated (middle) and outlined experimental versus simulated damage patches (right) under perturbed loading condition. Simulated damage contours and iso-lines are in 0.05 mm increments. Good agreement between the simulated and experimentally derived damage patches is indicated by similar perimeter shapes in the right image (simulated=solid, experiment=dots).

Force Comparisons

To determine the ability of the simulation to match the mechanics of the testing apparatus, simulated AP force and IE torque predictions were compared to those measured by the load cell in the Force 5\(\text{TM}\). Results are shown in Figure 3.24 for both load conditions. Table 1 summarizes the normalized root mean square (nRMS) prediction errors. nRMS values are the error divided by the total range of that data.
Figure 3.23: Experimentally observed (thin lines) versus simulated (thick lines) volumetric wear under original (round markers) and perturbed (square markers) loading conditions. Excellent agreement in terms of final volumetric wear and volumetric wear rate are observed for original loading conditions. Excellent agreement in terms of final volumetric wear is observed for perturbed loading conditions, although the volumetric wear rate differs.
measure (reported as a percentage). Overall, there was agreement between the data. Poorest representation occurred when simulating the AP forces at the end of the perturbed experiment, but general trends and magnitudes agree well.

Table 3.3: Normalized root mean square* error between simulation-predicted and experiment-mean force and torque measures. Data are normalized with respect to the total range of a given measure.

<table>
<thead>
<tr>
<th></th>
<th>Original Loading</th>
<th></th>
<th>Perturbed Loading</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>AP Force Error</td>
<td>IE Torque Error</td>
<td>AP Force Error</td>
<td>IE Torque Error</td>
</tr>
<tr>
<td>Start Finish</td>
<td>Start Finish</td>
<td>Start Finish</td>
<td>Start Finish</td>
<td>Start Finish</td>
</tr>
<tr>
<td>nRMS</td>
<td>8.3% 11.9%</td>
<td>7.2% 8.4%</td>
<td>12.7% 16.6%</td>
<td>14.4% 5.3%</td>
</tr>
<tr>
<td>Max Error</td>
<td>38.2% 40.0%</td>
<td>19.3% 22.8%</td>
<td>48.5% 53.7%</td>
<td>38.9% 14.4%</td>
</tr>
</tbody>
</table>

\[ nRMS = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (F_{\text{sim},i} - F_{\text{exp mean},i})^2 / \text{range} (F_{\text{exp mean}})} \]

3.5 Discussion

The comparison of experimentally measured versus simulation predicted AP forces and IE torques shows that the model predicts the experiment mechanics with reasonable accuracy (average error of 12.4% for forces, 12.4% for torques). It is interesting to note that the overall trend and magnitude of the simulated forces and torques are similar to the measured values, despite the fact that the quasi-static simulation is incapable of accounting for any dynamic or inertial effects. Frictional properties on the surface of the implant may have changed over time as burnishing and polymer reorientation occurred [28], contributing to larger errors at the end of the tests.

Almost twice as much wear was observed using the perturbed kinematics, in agreement with previous experimental findings [7, 108]. The direction of IE rotation was
Figure 3.24: Experimental versus simulated load cell forces and torques using (a) original test conditions: Simulation
Experiment mean +/- 2 standard deviations

(b) perturbed test conditions
Simulation
Experiment mean +/- 2 standard deviations

Figure 3.24: Experimental versus simulated load cell forces and torques using (a) original and (b) perturbed loading conditions. Good agreement in terms of trends and magnitudes are observed for most measures.
reversed, but was not believed to contribute to any change in volumetric wear due to symmetry at the contacting surfaces. The magnitude of IE rotation was approximately twice that of the original loading condition so more crossing motion (lower $\beta$) was present under the perturbed condition (Fig. 3.25a), increasing wear (Fig. 3.25b). This behavior could only be matched with a wear model which accounted for the effects of strain hardening, which the traditional Archard’s wear model does not take into account.

(a) Crossing motion $\sigma = 1 - \beta$ (0.005 increments)

(b) Wear (0.025 mm increments)

Figure 3.25: Amount of crossing motion (a) and wear (b) after original and perturbed loading. Both are increased significantly under the perturbed loading due to higher IE rotations.

The tuned model predicted nearly identical volumetric wear under perturbed loading conditions as measured experimentally. One concern is the discrepancy in the
rate of volumetric wear under perturbed loading. Experiment measurements show a slightly higher volumetric wear rate than the numerical simulation, which could lead to disagreements in volumetric wear beyond 3.5 million cycles. The RMS error when considering all matched data points is $4.5 \text{ mm}^3$ (9.2\% final volume). Considering the significant uncertainties which can arise during wear measurement due to moisture / protein uptake, contamination of samples and balance accuracy, the prediction is within an acceptable range.

The size and distribution of the damage patches caused by the original versus perturbed loadings were observed to be quite different, while similarities between the measured damage patch and the respective simulated damage were easily identified. The accuracy of laser scanner measurements is questionable; however they do give an accurate measure of the relative (rather than absolute) damage distribution across the surfaces. The small discrepancies between simulated and measured damage depths, therefore, are of little concern. The size and shape of the damage patch was of greater interest and indeed in agreement with the simulated damage. This indicated that the location of damage was being simulated correctly, although the extent of damage could not be verified directly using this approach alone.

The strength of the model at predicting both original and perturbed wear testing results validates the following assumptions which went into the model: Based on the model by Wang [28] and findings of Turell at al. [22] it was assumed that frictional work expended along the polymer molecules would not produce any wear, while frictional work expended perpendicular to molecules would. It was also assumed that the actual contact surface composition can be approximated by a fully aligned (strain hardened) fraction and a completely multidirectional fraction. Further experiment,
especially pin-on-disk testing, would be beneficial in testing these assumptions. Ideally, similar experiments to those of Turell et al. [22] should be performed, with higher cycle counts, more wear patterns and more samples.

Testing the validity of the particular model when applied to highly crosslinked UHMWPE is another possible direction for future work. The presence of stronger crosslinks is believed to resist the molecular reorientation which causes strain hardening [7, 28], keeping $\beta$ close to zero. If this is indeed the case, the current model would require a second material parameter to associate frictional work to the amount of strain hardening. If the strain hardening phenomenon is completely prevented by strong crosslinking, the classic Archard and Hirst model [42] might be preferred for its simplicity. The experimental work of Kang et al. [23, 105], however, showed that cross shear caused an increase in wear for both conventional and highly crosslinked UHMWPE.
Chapter 4

Kinematics

A kinematics objective function was required for the computational framework. Before a numerical kinematics simulation could be implemented as a performance measure, it was first necessary to tune some model parameters and ensure that the simulator was capable of duplicating real experimental results. This chapter describes the kinematics experiments and simulations being tuned / validated.

4.1 Kinematics Experiment

The kinematics experiments performed for model validation measured two different types of performance data. Laxity experiments measured the constraint of the TKR design. In these experiments, an axial load was applied between the femoral and tibial components, the tibial component being semi-constrained, and then anterior-posterior displacements or internal-external rotations were applied. The resulting forces and torques can be used as a measure of implant constraint or laxity. Unconstrained flexion kinematics experiments measured the relative femorotibial kinematics when
the tibial component is essentially unconstrained and the femoral component is flexed or extended.

### 4.1.1 Apparatus

**Force 5**\textsuperscript{TM} for Kinematics

The kinematics experiments were performed using the same Force 5\textsuperscript{TM} simulator machine as described in 3.1.1. For the laxity experiments, the required implant components’ degrees of freedom were the same as described for wear simulation, so no modifications to the Force 5\textsuperscript{TM} were required. For the unconstrained flexion kinematics experiments, it was required that all tibial degrees of freedom be unconstrained, except for flexion-extension. This was achieved using a modified tibial base system (Figs. 4.1, 4.2 and 4.3), which consisted of an adduction-abduction revolute joint (using a pivot) and a planar joint (using ball bearings) installed onto the tibial axial load cylinder. The planar joint provided a very low friction surface for AP and ML displacements and IE rotations.

The fluid handling system was not used for kinematics experiments, and implant surfaces were lubricated with grease rather than a bovine serum solution.

**Optotrak**\textsuperscript{TM} for Motion Tracking

During laxity experiments, forces were measured by the load cell and displacements were prescribed, so all experimental data was recorded by the Force 5\textsuperscript{TM} itself. During unconstrained flexion kinematics experiments, however, the UHMWPE insert was unconstrained while flexion-extension was applied to the femoral component. The Force 5\textsuperscript{TM} had no means of measuring UHMWPE insert kinematics, so an
CHAPTER 4. KINEMATICS

Figure 4.1: Depiction of modified tibial base system used to provide unconstrained degrees of freedom to the insert component during flexion tests. AA rotation is provided by a pivot along the distal surface of the insert component. ML and AP displacements and IE rotations are provided by a planar (ball bearing) joint.

Figure 4.2: Depiction of tibial base system to provide unconstrained degrees of freedom to the insert, as a frontal plane cross section view. The configuration of the pivot and ball bearing joints are indicated.
Optotrak™ Certus™ (Northern Digital Inc., Waterloo, Ont) motion tracking system was used to track that component (Fig. 4.4). The system uses a camera to track the position of infrared markers (iReds) in three dimensions with 0.1 mm accuracy at a 0.01 mm resolution. A rigid body with four mounted iReds (Fig. 4.5) was attached to the UHMWPE insert component of the TKR, allowing us to track the position and orientation with respect to a global reference frame.

**Samples**

Several different designs needed to be tested in order to ensure that the experiment and simulation could achieve matching results regardless of the implant shape. While different commercial implants could have been used, most designs are quite similar in terms of contact surface geometry when considering posterior cruciate sacrificing
Figure 4.4: Optotrak\textsuperscript{TM} Certus\textsuperscript{TM} camera capable of tracking infrared marker positions in three dimensions with 0.1 mm accuracies. The camera tracked markers attached to the unconstrained insert component during flexion tests.

Figure 4.5: iRed rigid body to provide motion tracking of insert components during flexion tests. Each marker can be tracked with 0.1 mm accuracy in three dimensions. The rigid body attached to a rod extending anteriorly from the insert components.
condylar total knees. While a parametric TKR modeller had been developed, the ability to make prototypes from actual implant materials (CoCr and UHMWPE) was not available. Instead, prototypes had to be printed from acrylonitrile butadiene styrene (ABS) plastic using a rapid prototyping machine. In order to determine if ABS plastic implant components could match the kinematics of CoCr-UHMWPE implants, an actual DePuy™ PFC Sigma™ (cruciate retaining, size 3, 8 mm) femoral component and UHMWPE insert (sample named “DePuy™-CoCr/UHMWPE”) were compared to a prototype with the exact same femoral and insert component geometry, but printed out of ABS plastic (sample named “DePuy™-ABS”). Three more samples with different geometries were randomly selected and also printed from ABS plastic (samples named “Design-A-ABS”, “Design-B-ABS”, and “Design-C-ABS”). The shape and conformity characteristics of the DePuy™ and randomly selected designs are depicted in Figures 4.6. Numerical models of each design were also generated for use in simulations, and are also shown in Figure 4.6 and denoted “DePuy™-STL”, “Design-A-STL”, “Design-B-STL”, and “Design-C-STL”.

The printed ABS plastic samples featured a protrusion running anteriorly to posteriorly along the distal (bottom) surface of the insert component. This protrusion sat in a groove above the planar joint and acted as a pivot to allow adduction-abduction rotation during unconstrained kinematics experiments. The component printing process produced a grained surface finish due to the method of ABS plastic extrusion. Surfaces with isotropic friction properties were required, so the components’ contact surfaces were sanded to a smooth finish. To accommodate the iRed rigid body for motion tracking, a 3 inch length of 3/16th of an inch drill-rod was inserted into the anterior face of the inserts so as to protrude parallel to the adduction-abduction axis.
### Figure 4.6: Implant designs used for kinematics experiments and simulations. Geometry was based on either actual DePuy™ components or randomly generated TKR designs.

<table>
<thead>
<tr>
<th>Design</th>
<th>Conformity</th>
<th>Experiment Components</th>
<th>Virtual Components</th>
<th>Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>DePuy™</td>
<td>medial lateral sagittal conformity at 0° flexion frontal conformity at 0° flexion frontal conformity at 90° flexion</td>
<td>DePuy™-CoCr/UHMWPE Design-A-ABS</td>
<td>DePuy™-STL DePuy™-ABS Design-A-STL</td>
<td>DePuy™-CoCr/UHMWPE versus DePuy™-ABS versus DePuy™-STL</td>
</tr>
<tr>
<td>Design-A</td>
<td>medial lateral sagittal conformity at 0° flexion frontal conformity at 0° flexion frontal conformity at 90° flexion</td>
<td>Design-B-ABS Design-C-ABS</td>
<td>Design-B-STL Design-C-STL</td>
<td>Design-B-ABS versus Design-B-STL Design-C-ABS versus Design-C-STL</td>
</tr>
<tr>
<td>Design-B</td>
<td>medial lateral sagittal conformity at 0° flexion frontal conformity at 0° flexion frontal conformity at 90° flexion</td>
<td>Design-C-ABS</td>
<td>Design-C-STL</td>
<td>Design-C-ABS versus Design-C-STL</td>
</tr>
</tbody>
</table>
The rigid body could be attached to this rod with a pair of set screws.

4.1.2 Loading

Laxity Experiment Loading

Loading for the laxity experiment was based on ASTM standard F 1223-05 [89]. An axial load of 710 N was applied through the tibial component while the femoral component was held fixed at 0° or 80° of flexion. Anterior-posterior displacements (+/-6.35 mm) of the femoral component and internal-external rotations (+/-10°) of the tibial component were applied as sinusoidal waveforms (rather than abrupt changes in motion) in lieu of the the forces applied in the ASTM standard, due to the limitations of the displacement-controlled Force 5™. No simulated soft tissue restraints or springs were applied. Waveform frequencies between 0.1 Hz and 0.5 Hz were tried, and finally a frequency of 0.25 Hz was chosen. At this rate, the motion was fast enough to minimize stiction effects caused by ABS-ABS contact but slow enough to ensure accurate reproduction of desired motions. The DOF status of the TKR components during anterior-posterior laxity and internal-external rotation laxity experiments are shown in Table 4.1.

Unconstrained Flexion Experiment Loading

Loading during the unconstrained flexion kinematics experiment was designed to determine what the relative femorotibial kinematics of a TKR design would be under axial load with flexion applied. Of particular importance were the amounts of anterior-posterior translation and internal-external rotation as functions of flexion. Since these motions are seen during flexion of the natural knee (femoral rollback and
internal rotation of the tibia), it was important to provide a situation where these motions (or lack thereof) could be observed in candidate TKR designs. The experiment included an axial load of 710 N, and femoral flexion applied as a sinusoidal wave between 0° and 80° at 0.25 Hz. No simulated soft tissue restraints or springs were applied. Aside from flexion-extension, all tibial degrees of freedom were unconstrained leaving the component free to move as a function of flexion angle and axial load (Table 4.2).

Table 4.2: Status of TKR component DOFs when installed on Force 5™ for unconstrained flexion kinematics simulations.

<table>
<thead>
<tr>
<th>TKR DOF</th>
<th>Femoral</th>
<th>Tibial</th>
</tr>
</thead>
<tbody>
<tr>
<td>Medial-lateral</td>
<td>Fixed</td>
<td>Free</td>
</tr>
<tr>
<td>Anterior-posterior</td>
<td>+/- 6.35 mm</td>
<td>Fixed</td>
</tr>
<tr>
<td>Proximal-distal</td>
<td>Fixed</td>
<td>710 N</td>
</tr>
<tr>
<td>Flexion-extension</td>
<td>0° or 80°</td>
<td>Fixed</td>
</tr>
<tr>
<td>Adduction-abduction</td>
<td>Fixed</td>
<td>Free</td>
</tr>
<tr>
<td>Internal-external</td>
<td>Fixed</td>
<td>0°</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Fixed  +/- 10°</td>
</tr>
</tbody>
</table>

Table 4.1: Status of TKR component DOFs when installed on Force 5™ for laxity simulations.

<table>
<thead>
<tr>
<th>TKR DOF</th>
<th>AP Laxity</th>
<th>IE Laxity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Femoral</td>
<td>Tibial</td>
<td>Femoral</td>
</tr>
<tr>
<td>Medial-lateral</td>
<td>Fixed</td>
<td>Free</td>
</tr>
<tr>
<td>Anterior-posterior</td>
<td>+/- 6.35 mm</td>
<td>Fixed</td>
</tr>
<tr>
<td>Proximal-distal</td>
<td>Fixed</td>
<td>710 N</td>
</tr>
<tr>
<td>Flexion-extension</td>
<td>0° or 80°</td>
<td>Fixed</td>
</tr>
<tr>
<td>Adduction-abduction</td>
<td>Fixed</td>
<td>Free</td>
</tr>
<tr>
<td>Internal-external</td>
<td>Fixed</td>
<td>0°</td>
</tr>
</tbody>
</table>
4.1.3 Experiment Protocol

The femoral component for a particular design was installed onto the femoral component holder on the Force 5™. For laxity experiments, the wear testing tibial component holder was mounted and the appropriate insert component was installed. Axial load was applied in low-pressure mode until contact between the components occurred, when the Force 5™ was then switched into high-pressure mode for more precise actuator control. The anterior-posterior position of the femoral component was adjusted such that the lowest contact points on the femoral condyles rested in the lowest possible points on the contact surface of the insert (laxity neutral point). For designs which featured a flat area, where the lowest points were ambiguous, a reasonably well centred position was chosen and noted so as to be reproduced accurately in simulations. Once components were aligned, cyclic laxity testing for AP displacements and IE rotations was performed using the loading described in 4.1.2. Load cell data was recorded for 20 seconds (5 cycles) during each experiment. An AP and then IE laxity experiment was performed at 0° flexion and then both repeated at 80°. This process was repeated 3 times for each implant design. Care was taken before each test to ensure that the axial load was correct and all other DOF were at their correct reference positions.

After the laxity experiment was complete, the axial load was removed and the implant components separated. The tibial component holder was removed and replaced by the modified tibial base system described in 4.1.1. The insert component was installed on the modified base, and axial load was reapplied in low-pressure mode until contact between the components was established.

The iRed rigid body had to be installed onto the 3 inch drill-rod protruding from
the anterior surface of the insert. Before installation, however, the rigid body was held flush against the Force 5™ femoral component holder, lying parallel to the sagittal plane. The position was recorded by the Optotrak™ in order to provide a reference coordinate system for subsequent measurements. This was repeated for each implant design, as the position of the Force 5™ with respect to the Optotrak™ could have changed between experiments. The rigid body was then attached to the insert to provide motion tracking. A square was used to align the insert at 0° IE rotation with respect to the femoral component, and the position was recorded to provide a reference of the iRed rigid body position with respect to the insert position in case of slight misalignment between the two. The testing apparatus prepared for unconstrained flexion experiments is shown in Figure 4.7.

Figure 4.7: Force 5™ testing apparatus configured for unconstrained flexion experiments. The iRed rigid body is installed onto the insert component in order to track the unconstrained motions.
Unconstrained flexion experiments under 710 N of axial load were performed (loading described in 4.1.2). Data was sampled at the same rate by both the Force 5\textsuperscript{TM} and Optotrak\textsuperscript{TM} (30 Hz) for a 20 second interval (5 cycles). The experiment was repeated 3 times for each implant design. Since the Force 5\textsuperscript{TM} sampled the last 20 seconds of data, while the Optotrak\textsuperscript{TM} sampled the next 20 seconds of data, careful timing was required to best align the two data sources. Alignment was not guaranteed and had to be addressed during post-processing. Once unconstrained flexion experiments were complete, the axial load was removed, the implant components were removed, and the next design could be tested.

The laxity and unconstrained flexion experiments were also performed using the CoCr-UHMWPE DePuy\textsuperscript{TM} design components. The same procedure was followed as above, except a holder for the UHMWPE insert had to be fabricated to provide the adduction-abduction pivot during unconstrained flexion experiments and a means for installing the iRed rigid body.

4.1.4 Data Management

The AP displacement and AP force during AP laxity experiments were recorded. The IE rotation and IE torque during IE laxity experiments were recorded. The three 20 second samples from each experiment were combined.

The femoral flexion angle was recorded by the Force 5\textsuperscript{TM} during unconstrained flexion experiments. The position and orientation of the insert with respect to the Force 5\textsuperscript{TM} could be calculated based on the positions of the rigid body’s iRed markers. While the complete three-dimensional position and rotation matrices of the insert
were calculated, only the AP displacements were of interest for the validation experiments. Since the flexion and AP displacement data were recorded from two different sources for the same experiment, some alignment of the data points were necessary. The data were aligned under the assumption that anterior displacement of the insert stopped when the femoral component reached maximum flexion, at which point extension began, accompanied by posterior displacement of the insert. This assumption was based on visual observations made during experiments and computational simulations. The three 20 second samples for each experiment were combined.

4.2 Kinematics Simulation

4.2.1 Rigid Body Models

STL Meshes

All of the implant components used for kinematics simulations were first modelled as a finite element mesh, either from available CAD geometry or using a parametric modeller which is described in the next chapter. A routine was coded that accepted a FE mesh of a component and converted the mesh to a surface mesh of triangles. This type of mesh is very similar to the standard tessellation language (STL) files used for stereolithography, which is a file format suitable for importing the model components into the rigid body dynamics solver MSC.Adams™ (MSC.Software Corporation, Santa Ana, CA). An ASCII STL file was easily translated from the FE triangle surface mesh for each component. In the FE and STL models, the average edge length of each triangle was approximately 2 mm. No STL mesh refinement study was performed, mesh size was instead selected for agreement with the FE models
used during wear experiments. The numerical models of each design (DePuy™-STL, Design-A-STL, Design-B-STL and Design-C-STL) are depicted in Figure 4.6.

**Force 5™ Modelling**

A model was constructed in MSC.Adams™ which provided the same testing conditions and degrees of freedom as the actual kinematics experiments. Since the apparatus was modified to provide different conditions for the laxity versus unconstrained flexion experiments, two models were created and simulations were performed separately.

For the laxity model, a femoral component holder with flexion-extension and anterior-posterior displacement degrees of freedom was created. A tibial component holder was modelled using a combination of a cylindrical joint (for internal-external rotation and axial load), a revolute joint (for adduction-abduction), and lastly a prism / translational joint for medial-lateral displacement between the insert component and the revolute joint.

For the unconstrained kinematics model, the same femoral component holder properties were used. For the tibial component holder, the cylindrical joint was used again but rotation was constrained. A planar joint was placed above the cylindrical joint, providing medial-lateral and anterior-posterior displacements, and internal-external rotations. Lastly, a revolute joint was modelled between the insert and the planar joint to provide and adduction-abduction degree of freedom.

Implant component STL files were imported into the model and positioned with respect to the femoral and tibial component holders. Positioning during the simulations was crucial, and precise measurements were taken to ensure agreement with the
experimental positioning.

**Contact Modelling**

Contact was modelled between the femoral and insert components. Unlike the FE simulations for wear, neither component was deformable. In FE contact analysis, minimizing penetration ensures model accuracy, and contact stiffness is a function of the compliance of the underlying deformable mesh. When modelling rigid-rigid contact, the contact stiffness must be provided explicitly as there is no material compliance information. Contact analysis in MSC.Adams™ using an Augmented Lagrange impact algorithm requires values for the:

- Stiffness
- Force Exponent
- Damping
- Penetration Depth
- Friction Parameters

Insufficient material property data was available to properly characterize the printed ABS plastic, so the values were instead tuned using a systematic optimization method in order to match experimental results.

### 4.2.2 Rigid Body Simulations

The loadings for laxity or unconstrained flexion kinematics simulations were applied to the components during simulations. Simulation durations were 20 seconds, each
performed using a minimum of 4000 iterations. If contact analysis required smaller
time increments, more iterations were performed automatically. The second-order
Hilber-Hughes-Taylor (HHT) solver was used with an error tolerance of 1E-5. The
priority of the HHT integrator is speed before accuracy, but with a small error toler-
ance acceptable accuracy is still maintained [109]. Trial simulations showed that the
HHT integrator was generally more successful at solving TKR contact problems than
the default Gear stiff integrator in MSC.Adams\textsuperscript{TM} (less simulation failures).

Following the simulations, the results file was processed in order to store the
relevant data for the laxity and unconstrained flexion kinematics simulations. For
AP and IE laxity, this was the AP displacements and AP forces or IE rotations and
IE torques, respectively. For unconstrained flexion kinematics, the flexion angles and
AP displacements were recorded.

4.3 Kinematics Experiment versus Simulation

4.3.1 Comparison Method

Laxity experiments and simulations yielded force versus displacement curves and
torque versus rotation curves for each design at 0\textdegree and 80\textdegree flexion. Unconstrained
flexion experiments and simulations yielded displacement versus flexion curves for
each design. Due to friction and the cyclic nature of the experiments, the data
formed hysteresis loops when plotted (Fig. 4.8). An automated method had to
be coded to compare experimental data (DePuy\textsuperscript{TM}-CoCr/UHMWPE implants ver-
sus DePuy\textsuperscript{TM}-ABS implants) and experiment versus simulation data (DePuy\textsuperscript{TM}-ABS
versus DePuy\textsuperscript{TM}-STL). This was accomplished by representing loops by three curves.
The slope curve $\chi$ was the average Y-axis values within a given X-axis window. The ceiling curve $\gamma$ was the highest Y-axis value within a given X-axis window, and the floor curve $\lambda$ was the lowest.

Figure 4.8: Extracting slope, ceiling and floor from loop for analysis. Extracting three curves allowed easier comparison between two hysteresis loops.

Separating the data in this manner allowed for two samples of data to be compared in two different ways. Error between the slope curves of two sample loops generally indicated different stiffnesses, caused by contact stiffness, Force 5™ compliance or different geometries. Error between the ceiling and floor curves of two sample loops generally indicated that friction was not being accounted for properly. This information better directed corrective action through manual and automated (optimization) tuning methods.

There were small inaccuracies in identifying the exact position of the insert relative to the Force 5™ reference frame when unconstrained flexion data were compared. This could be addressed by offsetting the AP displacements to better align the slope curves for two samples. This was done automatically using early flexion data (see Fig. 4.9). The total AP displacements, however, were unaffected by this offset.

The total slope or stiffness error $\epsilon_s$ is calculated as the normalized RMS error (eq. 4.1) between the two $\chi$ curves (eq. 4.2). The total hysteresis or friction error $\epsilon_f$ is
Figure 4.9: Comparing two data loops (solid and dotted), an offset was sometimes present due to AP reference position errors. Removing offset from AP displacements minimized the effect of these errors. Only early flexion data was compared for alignment. Overall AP displacement magnitudes were not affected.

calculated as normalized RMS error between the two $\gamma$ and $\lambda$ curves (eq. 4.3). The overall error $\epsilon_{\text{tot}}$ of one loop to another is calculated as the RMS of the stiffness and friction errors (eq. 4.4).

\[
n \text{RMS} (A, B) = \sqrt{ \frac{1}{n} \sum_{i=1}^{n} (A_i - B_i)^2 } \quad \text{range} (A) \quad \text{(4.1)}
\]

\[
\epsilon_{s} (\alpha, \beta) = n \text{RMS} (\chi_\alpha, \chi_\beta) \quad \text{(4.2)}
\]

\[
\epsilon_{f} (\alpha, \beta) = \sqrt{ \frac{n \text{RMS} (\gamma_\alpha, \gamma_\beta)^2 + n \text{RMS} (\lambda_\alpha, \lambda_\beta)^2}{2} } \quad \text{(4.3)}
\]

\[
\epsilon_{\text{tot}} (\alpha, \beta) = \sqrt{ \frac{\epsilon_{s} (\alpha, \beta)^2 + \epsilon_{f} (\alpha, \beta)^2}{2} } \quad \text{(4.4)}
\]
4.3.2 Results

Implant Materials: DePuy\textsuperscript{TM}-CoCr/UHMWPE versus DePuy\textsuperscript{TM}-ABS

The unconstrained flexion and laxity experiment results of the DePuy\textsuperscript{TM} implant geometry using actual implant components (DePuy\textsuperscript{TM}-CoCr/UHMWPE, red lines) versus ABS plastic copies (DePuy\textsuperscript{TM}-ABS, blue lines) are compared in Figure 4.10. The error scores for each comparison calculated using Equations 4.1–4.4 are shown in Table 4.3.

Table 4.3: Comparing DePuy\textsuperscript{TM}-CoCr/UHMWPE versus DePuy\textsuperscript{TM}-ABS components in terms of unconstrained flexion and laxity performance. Low error scores suggest that implant grade materials can be reasonably approximated using ABS plastic.

<table>
<thead>
<tr>
<th>Test</th>
<th>$\epsilon_s$</th>
<th>$\epsilon_f$</th>
<th>$\epsilon_{tot}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unconstrained Flexion</td>
<td>5.47</td>
<td>7.29</td>
<td>6.45</td>
</tr>
<tr>
<td>AP Laxity, 0°</td>
<td>2.75</td>
<td>3.47</td>
<td>3.13</td>
</tr>
<tr>
<td>AP Laxity, 80°</td>
<td>4.34</td>
<td>5.01</td>
<td>4.69</td>
</tr>
<tr>
<td>IE Laxity, 0°</td>
<td>2.60</td>
<td>3.20</td>
<td>2.92</td>
</tr>
<tr>
<td>IE Laxity, 80°</td>
<td>5.11</td>
<td>5.40</td>
<td>5.25</td>
</tr>
</tbody>
</table>

Tuning Kinematics Model using DePuy\textsuperscript{TM}-ABS versus DePuy\textsuperscript{TM}-STL Results

Laxity and unconstrained flexion simulations had parameters which required tuning, because default values provided by MSC.Adams\textsuperscript{TM} were not appropriate for ABS plastic. These simulation parameters included contact algorithm parameters, friction properties and the stiffness of the Force 5\textsuperscript{TM}. Tuning was performed by comparing experiment to simulation results for the DePuy\textsuperscript{TM} geometry (DePuy\textsuperscript{TM}-STL versus...
Figure 4.10: Comparing unconstrained flexion performance (top) and laxities of DePuy\textsuperscript{TM}-CoCr/UHMWPE (red lines) versus DePuy\textsuperscript{TM}-ABS (blue lines) components.
DePuy\textsuperscript{TM}-ABS) and minimizing the overall error score $\epsilon_{\text{tot}}$. Parameters were first manually tuned, and then further refined using the \textit{fmincon} optimization program in Matlab\textsuperscript{TM}. Force 5\textsuperscript{TM} compliance, which was not originally modelled, was added to the simulation when it was suspected to be a factor limiting simulation accuracy. This was modelled by adding a rotational spring below the tibial component holder which simulated anterior-posterior bending of the axial load cylinder in the sagittal plane. The bending reduced the AP constraint force generated for a given AP displacement, and was necessary for matching experimental results. The initial versus tuned parameters are shown in Table 4.4. The error between the simulation results and the experiment results (DePuy\textsuperscript{TM}-STL versus DePuy\textsuperscript{TM}-ABS) before and after tuning are shown in Table 4.5. For plots of the simulation results compared to the experiment results before and after tuning, refer to Figures B.1–B.2 in Appendix B.

**Validating Tuned Model using Multiple Component Shapes**

After tuning the model, it was used to simulate three random designs (Designs-A-STL, -B-STL, and -C-STL). Matching experimental data for the three designs was also available (Design-A-ABS, -B-ABS, and -C-ABS). In these simulations / experiments, the AP translation during AP laxity testing was increased from +/-6.35 mm to +/-7.62 mm, as these designs featured greater AP laxity than the DePuy\textsuperscript{TM} design. The resulting errors of the simulation results compared to the experiment results are show in Table 4.6. Plots comparing the results for each test for each design are shown in Figures B.3–B.5 in Appendix B.
Table 4.4: Initial versus tuned kinematics simulation parameters. Force $5^\text{TM}$ stiffness was reduced from fully rigid to compliant in order to match experimental results.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial</th>
<th>Tuned</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact Stiffness [N/mm]</td>
<td>10,000</td>
<td>1635</td>
</tr>
<tr>
<td>Contact Damping [Ns/mm]</td>
<td>10</td>
<td>163</td>
</tr>
<tr>
<td>Maximum Penetration Depth [mm]</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>Force Exponent</td>
<td>2.2</td>
<td>1.19</td>
</tr>
<tr>
<td>$\mu_{\text{static}}$</td>
<td>0.4</td>
<td>0.067</td>
</tr>
<tr>
<td>$\mu_{\text{dynamic}}$</td>
<td>0.1</td>
<td>0.053</td>
</tr>
<tr>
<td>Stiction Transition Vel. [mm/s]</td>
<td>100</td>
<td>1</td>
</tr>
<tr>
<td>Friction Transition Vel. [mm/s]</td>
<td>1000</td>
<td>1</td>
</tr>
<tr>
<td>Force $5^\text{TM}$ Stiffness [Nmm/deg]</td>
<td>$\infty$</td>
<td>50595</td>
</tr>
</tbody>
</table>

Table 4.5: Initial and tuned DePuy$^\text{TM}$-STL kinematics simulations compared to DePuy$^\text{TM}$-ABS experiments. Overall errors for each kinematics test decreased after tuning.

<table>
<thead>
<tr>
<th>Test</th>
<th>Initial $\epsilon_{\text{tot}}$ [%]</th>
<th>Tuned $\epsilon_{\text{tot}}$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unconstrained Flexion</td>
<td>7.57</td>
<td>5.40</td>
</tr>
<tr>
<td>AP Laxity, 0°</td>
<td>19.74</td>
<td>3.20</td>
</tr>
<tr>
<td>AP Laxity, 80°</td>
<td>10.39</td>
<td>3.89</td>
</tr>
<tr>
<td>IE Laxity, 0°</td>
<td>9.60</td>
<td>2.94</td>
</tr>
<tr>
<td>IE Laxity, 80°</td>
<td>8.62</td>
<td>5.53</td>
</tr>
</tbody>
</table>
Table 4.6: The tuned model was used to simulate the kinematics of Design-A-STL, -B-STL, and -C-STL. The results are compared to matching experiments with Design-A-ABS, -B-ABS, and -C-ABS. Low overall error scores suggest that the tuned model sufficiently simulated the experimental conditions.

<table>
<thead>
<tr>
<th>Test</th>
<th>Design-A-STL</th>
<th>Design-B-STL</th>
<th>Design-C-STL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unconstrained Flexion</td>
<td>8.21</td>
<td>5.06</td>
<td>6.83</td>
</tr>
<tr>
<td>AP Laxity, $0^\circ$</td>
<td>4.22</td>
<td>7.37</td>
<td>6.15</td>
</tr>
<tr>
<td>AP Laxity, $80^\circ$</td>
<td>4.24</td>
<td>7.51</td>
<td>5.46</td>
</tr>
<tr>
<td>IE Laxity, $0^\circ$</td>
<td>11.13</td>
<td>9.67</td>
<td>8.15</td>
</tr>
<tr>
<td>IE Laxity, $80^\circ$</td>
<td>6.04</td>
<td>7.42</td>
<td>11.15</td>
</tr>
</tbody>
</table>

4.4 Discussion

4.4.1 Actual Implant Components versus ABS Plastic Copies

Comparing laxity for the actual DePuy$^\text{TM}$ implant components versus the ABS plastic copies (DePuy$^\text{TM}$-CoCr/UHMWPE versus DePuy$^\text{TM}$-ABS), good agreement was obtained for all laxity measurements. Overall error scores ranged between 2.92% and 5.25%, with the highest overall errors observed during the IE laxity experiments at $80^\circ$ flexion while the lowest overall errors observed during the IE laxity experiments at $0^\circ$ flexion. Comparing the unconstrained flexion experiment results, poorer agreement was observed, with an overall error of 9.44%.

Agreement appears to worsen with increased flexion, which prompted an investigation into the apparatus setup. It was determined that the installation of the femoral component onto the femoral component holder was likely the source of these disagreements. While the positioning of this component in the anterior-posterior direction was in good agreement using the two different implants, the vertical positioning with
respect to the holder differed by approximately 1.5 mm. This positioning error was due to the thickness of a layer of bone cement used on the DePuy™-ABS femoral component but not the DePuy™-CoCr/UHMWPE femoral component. This shifted the lowest point on the femoral condyles of the ABS component lower with respect to the centre of rotation of the Force 5™ flexion axis. As the femoral component was flexed, this caused further anterior displacement of the insert for the DePuy™-ABS implant compared to the actual DePuy™-CoCr/UHMWPE implant. This increased AP displacement can be observed in the unconstrained flexion comparison in Figure 4.10. This would also impact laxity values when the femoral component is flexed, causing the increased error values for AP and IE laxity at 80°.

Another source of disagreement between the two implants was “stiction” between the femoral component and insert for the DePuy™-ABS implant. The components stuck together during counterface changes in direction during the laxity experiments, until the static coefficient of friction was overcome. This was not observed in the actual implant components, and was probably due to both components being the exact same material for the ABS plastic copy. Increasing the cycle frequency helped to reduce this effect, as well as using a heavier lubricant (grease), however the problem could not be completely removed.

4.4.2 Simulations versus ABS Plastic Experiment Results

Once tuned parameters were identified using the systematic tuning optimization method, the DePuy™-ABS experiment results were simulated with much better accuracy using the DePuy™-STL model, with the minimum and maximum errors reducing from 7.57% and 19.74% intially to 2.94% and 5.53% once tuned. A major
contributor to the initial error was the coefficient of friction, which was found to be significantly different than the MSC.Adams\textsuperscript{TM} contact model defaults. Another contributor was modelling the compliance of the Force 5\textsuperscript{TM}, which was initially assumed rigid (infinite stiffness).

\subsection*{4.4.3 Validation of the Tuned Model}

The tuned model performed quite well, with overall error scores for simulating insert kinematics during unconstrained flexion ranging between 5.06\% and 8.21\%. Small amounts of friction in the planar joint on the Force 5\textsuperscript{TM} which was neglected in simulations and Optotrak\textsuperscript{TM} accuracy may have contributed to these errors. Simulating the AP and IE laxities, overall error scores ranged between 4.22\% and 11.15\%. The errors in predicting IE laxity results were consistently worse than AP laxity, possibly due to small errors in positioning the femoral component with respect to the femoral flexion axis. This positioning error was determined to be a major contributor to the difference between actual DePuy\textsuperscript{TM}-CoCr/UHMWPE and DePuy\textsuperscript{TM}-ABS kinematics, and it is likely that the exact positioning was not correctly reproduced in the simulations.

Generally, the shape and magnitudes of the simulated curves are in good agreement with the experimental results. These results validate the kinematics simulation framework, at least in terms of the contact modeller in MSC.Adams\textsuperscript{TM}. While agreement with ABS plastic component experiments was acceptable, it is believed that using actual implant components (and respective simulation parameters) would yield even smaller errors. The “stiction” effect which seemed to plague experimental results for the ABS plastic components was difficult for the simulation to match. This was
not observed with the actual DePuy\textsuperscript{TM}-CoCr/UHMWPE components, which should improve simulation agreement.
Chapter 5

Multiobjective Optimization of a TKR

5.1 Parametric Modeller

A parametric TKR model was required for design optimization. The different radii of curvature, thicknesses, and conformities between components all had to be parameterized in order to find the best possible design. The parametric modeller had to generate finite element meshes of implant components for wear simulations as well as identical STL CAD models of components for kinematics simulations. HyperMesh™ was used as the foundation of the parametric modelling framework. This program was chosen for its strong meshing capabilities. Hexahedral elements are ideal for FEA, but many FE pre-processors are only capable of hex-meshing the simplest of geometries. HyperMesh™, on the other hand, has many special techniques for hex-meshing even the most complicated geometries, such as TKR components.

Custom script was written for HyperMesh™ in the TCL/TK command language.
While HyperMesh™ is generally suited for use through a graphical user interface, the scripting language allows one to run the software in batch mode, although at a much limited capacity. The script contained instructions which enabled HyperMesh™ to construct TKR component models, mesh the models, define contact surfaces, and apply material properties. The script could be modified by Matlab™ in order to make changes to the TKR geometry and the resulting FE mesh. The mesh was suitable for FE analysis in ANSYS™, and the material properties were selected to match those of the commercial FE design simulated in 3.3.

Once the FE mesh was generated by HyperMesh™, a second step imported the mesh back into HyperMesh™ and stripped away all material information and internal mesh, leaving only surface meshes of the TKR components. The surface meshes were modified to consist of triangular instead of rectangular elements. While technically still a finite element mesh, the resulting triangle meshes were similar to the surface tessellation used in STL CAD files. Further scripting in Matlab™ converted the mesh into the STL format, suitable for rigid body dynamics analysis in MSC.Adams™.

Which features to parameterize and how much each could change had to be decided. Geometry that was not parameterized included the bone-implant interface of the femoral component and the transverse plane perimeter shape of the UHMWPE insert. These shapes influence the bone cutting required during implantation, and the amount of bone which needs to be resected. These shapes were chosen to match the corresponding geometries of typical commercial TKR designs. While these parameters do not directly influence the contact surface geometry, they limited how much the contact surface parameters could change (especially for the femoral component). The thickness of the UHMWPE insert was also held constant. It is expected that a
surgeon would select the appropriate thickness of an UHMWPE insert, rather than be forced to use one “optimal” thickness. The amount of damage at the UHMWPE contact surface is dominated by creep damage, which is directly proportional to the thickness of the UHMWPE insert (Eq. 2.2). The affect of thickness on volumetric wear was not studied, although it is known that high wear rates and catastrophic material failures are likely if the UHMWPE insert is too thin. It was also assumed that thickness would have no impact on implant kinematics.

Parameters were often found to be incompatible with one another, meaning changing them independently would cause modeller failures (geometry that was impossible to generate or impossible to mesh). In these cases, parameters were either coupled or fixed to a constant value. Other issues arose during simulations with the finite element or STL CAD models, which required limiting or fixing parameters for simulation stability.

The length of time design optimization requires to converge to an optimum design is directly related to the number of design variables and how much each design variable can change. Coupling or removing design variables for the reasons above actually improved optimizer performance, assuming the optimizer was not restricted from reaching the true optimum. Even after many design variables were coupled or fixed, there were still a greater number of design variables than is ideal for design optimization. More design variables were removed or limited to a smaller range by performing a series of sensitivity and correlation studies. Considering design variables which had little to no correlation with our performance measures would be inefficient, and those parameters were fixed to constant values. By the end, 14 design variables, each having a considerable correlation to wear or kinematics performance, remained
for consideration during optimization. These design variables are listed in Table 5.1.

The sagittal radii of curvature of the femoral condyles, along the distal and posterior edges were parameterized (Fig. 5.1), as well as the sagittal conformity with the UHMWPE insert (Fig. 5.2). The condyles were allowed to be asymmetric, like the natural knee and a design feature not often seen in TKR. The sagittal plane geometry was expected to contribute greatly towards both the wear and kinematics performance of TKR. In order to reduce the number of design variables, the anterior and posterior sagittal radii of curvatures for the UHMWPE insert were both defined as being equal to the femoral distal radius of curvature plus some unconformity (therefore, the anterior and posterior sagittal radii of the UHMWPE are always greater than or equal to the femoral distal radius of curvature).

![Figure 5.1: Sagittal plane femoral component geometry. Parameters control the different radii of curvature which combine to form the sagittal profile.](image)

Frontal plane geometry was expected to impact mostly on the wear performance (influencing contact area and contact pressure). The frontal radii of curvature of both femoral condyles were allowed to change independently (Fig. 5.3), as well as the conformity of the UHMWPE insert in the frontal plane (Fig. 5.4). The width between the medial and lateral contact points between the femoral component and
Table 5.1: Design variables controlling the shape of the parametric TKR model. Variables can be combined into a 14 dimension design vector for the parametric modeller.

<table>
<thead>
<tr>
<th>Design Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RDMed</td>
<td>Radius of curvature of medial distal femoral condyle in sagittal plane</td>
</tr>
<tr>
<td>RDLat</td>
<td>Radius of curvature of lateral distal femoral condyle in sagittal plane</td>
</tr>
<tr>
<td>RPMed</td>
<td>Radius of curvature of medial posterior femoral condyle in sagittal plane</td>
</tr>
<tr>
<td>RPLat</td>
<td>Radius of curvature of lateral posterior femoral condyle in sagittal plane</td>
</tr>
<tr>
<td>RFMed</td>
<td>Radius of curvature of medial femoral condyle in frontal plane</td>
</tr>
<tr>
<td>RFLat</td>
<td>Radius of curvature of lateral femoral condyle in frontal plane</td>
</tr>
<tr>
<td>WMed</td>
<td>Medial femoral condyle spacing</td>
</tr>
<tr>
<td>WLat</td>
<td>Lateral femoral condyle spacing</td>
</tr>
<tr>
<td>CSMed</td>
<td>Conformity of anterior and posterior curve of medial UHMWPE insert cup to medial distal femoral condyle in sagittal plane</td>
</tr>
<tr>
<td>CSLat</td>
<td>Conformity of anterior and posterior curve of lateral UHMWPE insert cup to lateral distal femoral condyle in sagittal plane</td>
</tr>
<tr>
<td>CFMed</td>
<td>Conformity of medial UHMWPE insert cup to medial femoral condyle in frontal plane</td>
</tr>
<tr>
<td>CFLat</td>
<td>Conformity of lateral UHMWPE insert cup to lateral femoral condyle in frontal plane</td>
</tr>
<tr>
<td>LMed</td>
<td>AP length of medial UHMWPE insert cup</td>
</tr>
<tr>
<td>LLat</td>
<td>AP length of lateral UHMWPE insert cup</td>
</tr>
</tbody>
</table>
CHAPTER 5. MULTIOBJECTIVE OPTIMIZATION OF A TKR

Figure 5.2: Sagittal plane UHMWPE insert component geometry. Parameters control the conformity of the insert with respect to the femoral component and the cup length along the AP direction.

UHMWPE insert was also parameterized, which was expected to affect kinematics (mostly in terms of IE laxity) and wear (influencing crossing motions).

Figure 5.3: Frontal plane femoral component geometry. Parameters control the radius of curvature of the frontal profile of each condyle, as well as the spacing along the ML axis.

The limits for each design variable were determined through numerical experiments testing hundreds of random designs. Limits were based on model / simulation stability, as well as wear / kinematics performance. The limits are shown in table 5.2. The limits on the UHMWPE insert geometry for the sagittal radii of curvature match those of the distal femoral radii of curvature (min 25 mm, max 50 mm). The same is
CHAPTER 5. MULTIOBJECTIVE OPTIMIZATION OF A TKR

Figure 5.4: Frontal plane UHMWPE insert component geometry. Parameters control the conformity with the femoral component.

true in the frontal plane (min 15 mm, max 60 mm). The limits for conformity, therefore, became a function of the maximum allowable value for an UHMWPE insert parameter and the current value of the corresponding femoral component geometry. This meant that conformity values lost meaning when the corresponding femoral component geometry reached its upper limit. For example, if RDMed = 50 mm, the sagittal radius of curvature of the UHMWPE insert medial condyle would be 50 mm, regardless of CSMed.

The overall parametric modeller computational framework is depicted graphically in Appendix C.

5.2 Wear Objective Function Evaluation

Simulation Simplifications

The validated wear simulation described in Chapter 3 was used as an objective function for wear during design optimization. Instead of the displacement controlled simulations which were developed through a combined numerical-experimental approach, it was possible to simply use the force controlled inputs described in ISO
Table 5.2: Upper and lower limits of the design variables controlling the shape of the parametric TKR model. During optimization, these limits are used to translate normalized values between 0 and 1 to actual design variable values.

<table>
<thead>
<tr>
<th>Design Variable</th>
<th>Lower Limit</th>
<th>Upper Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>RDMed</td>
<td>25 mm</td>
<td>50 mm</td>
</tr>
<tr>
<td>RDLat</td>
<td>25 mm</td>
<td>50 mm</td>
</tr>
<tr>
<td>RPMed</td>
<td>14 mm</td>
<td>20 mm</td>
</tr>
<tr>
<td>RPLat</td>
<td>14 mm</td>
<td>20 mm</td>
</tr>
<tr>
<td>RFMed</td>
<td>15 mm</td>
<td>60 mm</td>
</tr>
<tr>
<td>RFLat</td>
<td>15 mm</td>
<td>60 mm</td>
</tr>
<tr>
<td>WMed</td>
<td>20 mm</td>
<td>22.5 mm</td>
</tr>
<tr>
<td>WLat</td>
<td>20 mm</td>
<td>22.5 mm</td>
</tr>
<tr>
<td>CSMed</td>
<td>0 mm</td>
<td>50 mm - RDMed</td>
</tr>
<tr>
<td>CSLat</td>
<td>0 mm</td>
<td>50 mm - RDLat</td>
</tr>
<tr>
<td>CFMed</td>
<td>0 mm</td>
<td>60 mm - RFMed</td>
</tr>
<tr>
<td>CFLat</td>
<td>0 mm</td>
<td>60 mm - RFLat</td>
</tr>
<tr>
<td>LMed</td>
<td>5 mm</td>
<td>8.75 mm</td>
</tr>
<tr>
<td>LLat</td>
<td>5 mm</td>
<td>8.75 mm</td>
</tr>
</tbody>
</table>
14243-1 [40] directly, using springs to provide simulated soft tissue restraint. An FE model constructed using the parametric modeller was substituted into the FE analysis, instead of the DePuy™ implant FE model. Other changes were made to the model in order to improve computational efficiency, vastly reducing the time required for design optimization. One modification was to no-longer force a wear measurement every 500,000 cycles. Since these simulations were not being compared with experimental results, there was no need to match measurement rates. This meant that wear measurements and contact surface geometry updates were only performed when incremental creep or total damage depths exceeded their respective limits. These limits were increased in order to reduce the number of iterations during a single wear simulation, with the creep criterion increased from 0.1 mm to 0.3 mm and the total damage criterion increased from 0.15 to 0.4 mm. Volumetric wear and maximum damage depth at 3.5 million cycles ($W_{vol}$ and $\delta_{max}$) were simulated.

**Simulation Enhancements**

The post-processor was enhanced in order to include the fatigue damage ($D_{max}$) scoring system proposed by Sathasivam and Walker [38] which is described in 2.6.4. This model was not included in the original wear simulations because validation of this component was not considered feasible. The ability to provide some measure of the likelihood of fatigue damage, however, would be useful during the assessment of parametric TKR designs in design optimization.
Simulation Time

After the simplifications and enhancements described above, the typical duration of a single FE iteration with a parametric model was approximately 40 minutes. The number of actual FE iterations during a single wear simulation generally reached 7-8, requiring up to 5 hours. The quoted times are for simulations running on an AMD Opteron 8222 series 64-bit processor (dual-core, 3.0 GHz each) with 4 GB of ram on SuSE Linux.

The overall wear computational framework is depicted graphically in Appendix C.

5.3 Kinematics Objective Function Evaluation

The validated kinematics simulation framework described in Chapter 4 was used as an objective function for kinematics during design optimization. Several modifications were made to both the unconstrained flexion and laxity simulations in MSC.Adams™. Since actual implant materials were being simulated, the coefficients of static and dynamic friction were both changed to 0.04 [50, 55] (equal to one-another in order to avoid the stiction effect). Force 5™ compliance was also removed – modelling machine compliance was only necessary during validation to match experimental results.

Unconstrained Flexion Simulation Modifications

In the original unconstrained flexion simulations, the femoral component was rotated between 0° and 80° of flexion, and the resulting AP displacements were in agreement with experimental results. The relative AP displacements of the femoral component with respect to the UHMWPE insert factors largely into the maximum flexion angle
of a TKR. Having validated this aspect of the simulation, we could use a modified version of the unconstrained flexion simulation to estimate the maximum safe flexion angle for a TKR design. A CAD model of a human femur was obtained from the Biomechanics European Laboratory (BEL) Repository. This was included in the simulation simply to provide a reference to when the femur would impinge on the posterior edge of the UHMWPE insert (Fig. 5.5).

![Figure 5.5: TKR configured for simulation in MSC.Adams™. Simulated PCL contribution is provided by two nonlinear tension-only springs. A femur is included for detecting posterior impingement with the UHMWPE insert.](image)

Springs were also installed between the femoral component and UHMWPE insert in order to simulate the contributions of an intact PCL (Fig. 5.5). Two springs represented the anterior and posterior bundles of the PCL. The origin and insertion locations were estimated based on available geometry and published coordinate data [110], and published nonlinear stiffness properties were applied [74, 81, 83]. The length of each ligament in the model was known, but the free length ($L_0$) of the ligament had to be calculated as a function of the published initial reference strain, $\epsilon_i$ (-0.1 for the anterior and posterior PCL bundles), at 0° flexion. With $L_0$ known,
ligament tensile force could be calculated using Equations 5.1 and 5.2. If PCL contribution was to be neglected, \( \epsilon_i \) was set to -0.9, which ensured the ligament would remain slack throughout the simulation. The ligament stiffness model features a nonlinear region and a linear region which dominates after \( 2\epsilon_l \), which was a constant term \( (\epsilon_l = 0.03) \). The stiffness \( k \) for each ligament was 9000 N. A plot of the resulting force-strain relationship is depicted in Fig. 5.6.

\[
\epsilon = \frac{L - L_0}{L_0} \quad (5.1)
\]

\[
f = \begin{cases} 
\frac{1}{2} k \epsilon^2 / \epsilon_l, & 0 \leq \epsilon \leq 2\epsilon_l \\
k (\epsilon - \epsilon_l), & \epsilon > 2\epsilon_l \\
0, & \epsilon < 0
\end{cases} \quad (5.2)
\]

Figure 5.6: Force-strain curve for PCL ligament bundles. The stiffness is nonlinear until strains above 0.06, when the stiffness is assumed to be linear. The nonlinear zone represents the untangling of ligament fibers.

In the modified simulation, the UHMWPE insert was unconstrained as before, and the femoral component was rotated until either of the following stopping criteria:
1. Contact between the femur bone and the UHMWPE insert (impingement).

2. Loss of contact between either femoral condyle with its respective UHMWPE insert cup (sublaxation).

The simulation was performed with and without PCL contribution, with the maximum safe flexion angle for that TKR design reported as the average of the two simulations. The average overall AP and ML translations and IE rotation were also reported, along with the maximum PCL strain (when present) and the percentage change in maximum safe flexion when the PCL contribution was added or removed.

**Laxity Simulation Modifications**

AP and IE laxity simulations were performed on the candidate TKR designs at 0° and 30° of flexion. During these simulations, PCL contributions were included, as described in the previous section. These flexion angles were chosen in order to allow comparison with the natural knee laxity data published by Li et al. [74]. The AP and IE laxity curves at 0° and 30° of flexion are shown in Fig. 5.7 and the derived average constraint values are shown in Table 5.3. The overall AP and IE constraint for a TKR design were calculated (in N/mm and Nmm/deg), as well as the constraint about the laxity neutral point. The laxity neutral point was assumed to be the point where constraint forces or moments changed sign (direction), normally coinciding with the lowest contact point on the UHMWPE insert. Laxity simulations at 90° of flexion were also performed and while the results were not compared to any published values, the significance of the PCL contribution was measured.

The laxity performance for a TKR design was thus described by three values:
• \( err_{tot} \) – The AP and IE laxity percent error with respect to published values, considering entire AP and IE range at 0\(^\circ\) and 30\(^\circ\).

• \( err_0 \) – The AP and IE laxity percent error with respect to published values, considering AP and IE constraint about laxity neutral point at 0\(^\circ\) and 30\(^\circ\).

• \( var_{pel} \) – The percentage change in AP and IE constraint at 90\(^\circ\) when the PCL is added or removed.

An ideal TKR design in terms of AP and IE laxity would yield low values for all three values, minimizing the error compared to natural knee laxity and minimizing sensitivity to the PCL.

Table 5.3: Overall AP and IE constraint at 0\(^\circ\) and 30\(^\circ\) of flexion for a natural knee, derived from Li et al. [74] data. Constraint is lower in flexion when compared to the extended position.

<table>
<thead>
<tr>
<th></th>
<th>0(^\circ) flexion</th>
<th>30(^\circ) flexion</th>
</tr>
</thead>
<tbody>
<tr>
<td>AP Constraint [N/mm]</td>
<td>26</td>
<td>14</td>
</tr>
<tr>
<td>IE Constraint [Nmm/deg]</td>
<td>642</td>
<td>442</td>
</tr>
</tbody>
</table>

Simulation Time

The modified kinematics simulations normally took between 5–10 minutes on the same computer system as described for wear simulations, using up to 4 CPU’s in MSC.Adams\textsuperscript{TM}. Some designs, seemingly randomly, experienced difficulty during contact analysis iterations which greatly increased solver times. When this occurred, solve time could reach up to 1 hour, but varied significantly for each design.

The overall unconstrained flexion kinematics and laxity simulation computational frameworks are depicted graphically in Appendix C.
Figure 5.7: Natural knee AP and IE laxity characteristics at 0° and 30° of flexion. Data was obtained from Li et al. [74]. Optimization will try to adjust TKR geometry to reproduce these laxity characteristics.
5.4 Single Objective TKR Design Optimization

5.4.1 The Optimizer

The \textit{fmincon} function in Matlab\textsuperscript{TM}, which is a gradient based optimization program with the ability to handle equality and inequality constraints, was used as the optimizer. Some optimizer settings, such as finite differencing step sizes, were specified manually based on previous optimizer performance while others were left at their default values. The optimizer was provided an initial design guess ($\bar{x}_0$), in the form of a 14-dimension vector of values normalized between 0 and 1 (the 14 parameters identified in Table 5.1). This vector represented the shape of the candidate TKR design. From this initial starting point, the optimizer would follow objective function and constraint gradient data until a feasible optimum design was converged upon.

The optimizer’s ability to find the global optimum was limited by the selection of the initial design and the number of local minima. A single design iteration required at least 15 objective function evaluations (14 during the finite differencing stage for gradient estimation, and at least 1 evaluation during the design-step stage), and typically more than 10 design iterations were required before the optimizer converged at an optimum (considering wear or kinematics). Rather than waiting for an optimization to converge automatically, most optimizations were terminated manually when several design iterations failed to produce any improvement in the objective function, or the optimizer appeared to be converging at a known local minimum.

An unfortunate drawback of parametric modelling and running simulations in batch mode is that some designs may fail during simulation. Normally, some sort of user intervention could address the simulation and salvage some results, but this type
of intervention is impossible during optimization, nor is it feasible to develop code with enough error handlers to address every type of simulation failure. In the case of a simulation failure (during either wear or kinematics objective function assessment), the code was designed to return a vector of +Inf values. During the design-step stage, an objective function and constraint value of +Inf was interpreted as a very poor design. The optimizer would steer away from this region of the design space. While this could cause the optimizer to miss out on a potential optimum design, it was necessary for the optimizer to stay in areas of the design space where design performance could be assessed accurately. If +Inf values were returned during a finite differencing calculation, the objective function gradient for the design variable which was being assessed was set to zero. This helped to improve convergence by reducing optimizer overreactions to false gradient information caused by +Inf results data.

The overall optimization computational framework is depicted graphically in Appendix C.

5.4.2 Performance of a Typical TKR Design

Method

Before performing design optimization, the numerical frameworks for wear and kinematics simulations were used to assess the performance of a commercially available DePuy™ PFC Sigma™ cruciate retaining TKR. This design was used in Chapters 3 and 4 for model validation, so the virtual model had already been generated. The PFC Sigma knee has a long standing history of clinical success [111–113] and is a modification to the original PFC knee which reported 10 year survival rates between 93–97% [112]. The performance of this design was used as a benchmark against which
Results and Discussion

The wear simulation with the DePuy™ design predicted a volumetric wear ($W_{vol}$) of 16.82 mm$^3$ per 3.5 million cycles, with a maximum damage depth ($\delta_{max}$) of 0.48 mm and a fatigue damage score ($D_{max}$) of 66. The total damage distribution after 3.5 million cycles is depicted in Figure 5.8. Optimization attempted to yield a design with a lower $W_{vol}$ than the DePuy™ TKR design.

The kinematics simulation with the DePuy™ design predicted a maximum flexion angle ($flx_{max}$) of 127°, when impingement between the femur and posterior edge of the UHMWPE insert occurred (Fig. 5.9). This value can be compared to mean maximum flexion values for the same implant design reported in the literature between 119° and 125° [111, 113]. The overall laxity error compared to the natural knee ($err_{tot}$)
was 107%. The laxity error about the neutral laxity point compared to the natural knee \( (err_0) \) was 167%. The actual constraint values are outlined in Table 5.4. The importance of the PCL to knee laxity \( (var_{pcl}) \) was 71%. Optimization attempted to yield a design with a higher \( flex_{max} \) than the DePuy\textsuperscript{TM} TKR design, and lower values for \( err_{tot}, err_0, \) and \( var_{pcl} \). Reducing \( err_{tot} \) and \( err_0 \) would make the artificial knee constraint more similar to that of the natural knee. Reducing \( var_{pcl} \) would reduce the importance of the PCL to knee laxity, making ligament balancing a less critical aspect of the TKR procedure.

![127° of flexion at impingement](image)

Figure 5.9: Maximum flexion of 127° for the DePuy\textsuperscript{TM} design before impingement. Impingement occurs earlier when femoral rollback is restricted, which occurs because of the high sagittal conformity of the DePuy\textsuperscript{TM} design.

Table 5.4: Overall AP and IE constraint at 0° and 30° for the DePuy\textsuperscript{TM} design. In general, AP constraint is higher than for the natural knee, while IE constraint is lower.

<table>
<thead>
<tr>
<th></th>
<th>Overall</th>
<th>About Neutral Point</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0° flexion</td>
<td>30° flexion</td>
</tr>
<tr>
<td>AP Constraint [N/mm]</td>
<td>76</td>
<td>21</td>
</tr>
<tr>
<td>IE Constraint [Nmm/deg]</td>
<td>496</td>
<td>125</td>
</tr>
</tbody>
</table>
5.4.3 Wear Optimized TKR

Method

Single objective design optimization was performed considering volumetric wear after 3.5 million cycles ($W_{vol}$) as the objective function to be minimized. The maximum damage depth after 3.5 million cycles ($\delta_{max}$) was constrained to be less than 1 mm, and the maximum damage score ($D_{max}$) was constrained to be less than 150. The wear performance of a candidate TKR design was performed using the modified simulation described in 5.2.

Optimizer performance improves when objective function and design variable magnitudes are the same order of magnitude. A large random sampling of TKR wear performance resulted in volumetric wear values up to approximately 50 mm$^3$, so the wear objective function was defined as:

$$J_{wear}(\bar{x}) = \frac{W_{vol}(\bar{x})}{50}$$  \hspace{1cm} (5.3)

This normalized the objective function between 0 and 1, in agreement with the design variables. The mathematical problem statement for wear optimization is described in Equation 5.4.
Minimize \( J_{\text{wear}} (\bar{x}) = \frac{W_{\text{vol}} (\bar{x})}{50} \)

subject to:
\[
\begin{align*}
\delta_{\text{max}} (\bar{x}) & \leq 1 \text{ mm} \\
D_{\text{max}} (\bar{x}) & \leq 150 \\
\bar{x}_{\text{min}} & \leq \bar{x} \leq \bar{x}_{\text{max}}
\end{align*}
\] (5.4)

where \( W_{\text{vol}} \) is the volumetric wear after 3.5 million cycles, \( \delta_{\text{max}} \) is the maximum damage depth, and \( D_{\text{max}} \) is the maximum damage score. Initial designs were randomly chosen, provided they were feasible in terms of \( \delta_{\text{max}}, D_{\text{max}}, \) and \( W_{\text{vol}} \). Many initial designs were attempted in order to improve the likelihood of finding the global optimum. With each objective function requiring up to 5 hours, each design iteration required at least 75 hours, often longer due to a highly nonlinear design–objective function relationship. Typically, a single design optimization for wear would run between 3-4 weeks before converging or being terminated manually.

Multiobjective design optimization was being performed at the same time as single objective design optimization for wear. Aside from approximately 10 random initial designs being considered for wear optimization alone, many more designs were being considered for wear and kinematics. This meant that wear performance data was available for many more designs than just those being generated from the 10 optimization threads for wear. The wear performance of all designs were monitored, as it was possible that one of those other designs could perform better than those found through wear optimization, due to the presence of many local minima. If such a design
was identified, that design was used as a start point for a new wear optimization.

**Results**

The best design in terms of wear performance was found and is depicted in Figure 5.10. The geometry is described in terms of its dimensions in Table 5.5. The predicted volumetric wear after 3.5 million cycles was $7.27 \text{ mm}^3$, with a maximum damage depth of 0.58 mm and a damage score of 88. The predicted wear, creep, and total damage distribution is depicted in Figure 5.11.

![Figure 5.10: Optimum TKR design in terms of UHMWPE volumetric wear reduction. The design features a nearly flat ML profile in the frontal plane. This increases contact area and lowers contact pressure.](image)

**Discussion**

The performance of the wear optimized design can be compared to the commercially available DePuy™ implant used during wear model validation. Using the modified wear simulation framework, the DePuy™ design is expected to generate $16.82 \text{ mm}^3$ of volumetric wear after 3.5 million cycles, versus only $7.27 \text{ mm}^3 \approx (\approx 56.8\%)$ for the wear optimized design. The maximum total damage depth of 0.58 mm and damage
Table 5.5: Description of optimum TKR shape in terms of UHMWPE volumetric wear reduction. High frontal radii of curvature produce a flat ML frontal profile. Low sagittal plane conformity is present at the medial condyle.

<table>
<thead>
<tr>
<th>Femoral Component</th>
<th>Medial</th>
<th>Lateral</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frontal Radius</td>
<td>RFMed = 60.0 mm</td>
<td>RFLat = 51.0 mm</td>
</tr>
<tr>
<td>Condyle Spacing</td>
<td>WMed = 20.9 mm</td>
<td>WLat = 20.7 mm</td>
</tr>
<tr>
<td>Distal Sagittal Radius</td>
<td>RDMed = 33.0 mm</td>
<td>RDLat = 40.8 mm</td>
</tr>
<tr>
<td>Posterior Sagittal Radius</td>
<td>RPMed = 20.0 mm</td>
<td>RPLat = 18.6 mm</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>UHMWPE Insert</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Frontal Radius</td>
<td>RFMed+CFMed = 60.0 mm</td>
<td>RFLat+CFLat = 52.8 mm</td>
</tr>
<tr>
<td>– unconformity</td>
<td>CFMed = 0 mm</td>
<td>CFLat = 1.8 mm</td>
</tr>
<tr>
<td>Sagittal Radius</td>
<td>RDMed+CSMed = 49.9 mm</td>
<td>RDLat+CSLat = 42.3 mm</td>
</tr>
<tr>
<td>– unconformity</td>
<td>CSMed = 16.9 mm</td>
<td>CSLat = 1.6 mm</td>
</tr>
<tr>
<td>Cup Length</td>
<td>LMed = 5.4 mm</td>
<td>LLat = 6.8 mm</td>
</tr>
</tbody>
</table>

Figure 5.11: Resulting wear, creep, and total damage distribution iso lines and contours (0.05 mm increments) for the wear optimized design. Wear damage is almost negligible when compared to the contribution of creep damage. Low wear damage results from low contact pressures, shorter sliding distances and reduced crossing motions.
score of 88, however, are greater than the DePuy™ design (0.48 mm and 66, respectively). The DePuy™ design has very high conformity in both the frontal and sagittal planes, reducing contact pressure as well as relative femorotibial translations. The increased damage depth is likely due to creep, which is proportional to the contact pressures and the thickness of the UHMWPE insert, both of which would be higher for the optimum design. The increased damage score is likely due to the lower medial sagittal conformity of the optimum design, allowing larger AP translations and stress fluctuations.

5.4.4 Kinematics Optimized TKR

Method

Single objective design optimization of a TKR was performed, considering unconstrained flexion kinematics and laxity characteristics. The modified simulations described in 5.3 were coupled with the parametric modeller and the optimization program, and an objective function was derived which assumed implant kinematics performance is a function of the maximum allowable flexion ($flex_{max}$), the overall match of AP and IE laxity characteristics to those of the natural knee ($err_{tot}$ and $err_0$), and the importance of the PCL to knee laxity ($var_{pcl}$). The optimizer sought to increase flexion, reduce the difference between the TKR and natural knee laxities, and reduce the impact of the PCL on knee laxity at 90° of flexion (in order to reduce the impact of ligament balancing on surgical outcome). The objective function was formed as a weighted sum of these performance measures.

While the kinematics simulation times alone were normally less than 10 minutes, wear performance was also calculated for every candidate design, making optimization
times on par with the single objective wear optimizations. This was because the wear constraints, $\delta_{\text{max}}$ and $D_{\text{max}}$, were also considered during kinematics optimization. Ensuring feasibility of the optimum design in terms of the wear constraints meant that the kinematics optimized design would be a feasible anchor point for multiobjective optimization. There were no constraints on kinematics performance.

Random initial designs were used as start points for the optimizer. Similar to during wear optimization, multiobjective optimization considering wear and kinematics was being performed in parallel with the kinematics optimization. The best performing designs in terms of kinematics were taken from that pool of results and used as initial designs for kinematics optimizations.

The kinematics performance measures had to be normalized to a comparable order of magnitude. A large random sampling of kinematics performances resulted in $\text{flex}_{\text{max}}$ values between approximately $100^\circ$ and $140^\circ$. Values for $\text{err}_{\text{tot}}$, $\text{err}_0$, and $\text{var}_{\text{pel}}$ were between 0 and 1. The $\text{flex}_{\text{max}}$ values were divided by $120^\circ$ to match the order of magnitude of the other values and the design variables. The entire objective function was divided by 2, in order to normalize the objective function magnitude to the same range as the design variables (between 0 and 1). The resulting mathematical problem statement for kinematics optimization was:
Minimize $J_{kin}(\bar{x}) = \left[ -\frac{flex_{max}(\bar{x})}{120} + err_{tot}(\bar{x}) + err_0(\bar{x}) + var_{pcl}(\bar{x}) \right]/2$

subject to:

\[
\begin{align*}
\delta_{max}(\bar{x}) & \leq 1 \text{ mm} \\
D_{max}(\bar{x}) & \leq 150 \\
\bar{x}_{min} & \leq \bar{x} \leq \bar{x}_{max}
\end{align*}
\]  

(5.5)

where $flex_{max}$ is the maximum flexion angle, $err_{tot}$ is the overall laxity error, $err_0$ is the neutral point laxity error, and $var_{pcl}$ is the importance of the PCL.

Results

The best design in terms of kinematics performance was found and is depicted in Figure 5.12. The geometry is described in terms of its dimensions in Table 5.6. The predicted maximum safe flexion angle ($flex_{max}$) is 143°, with $err_{tot}$ and $err_0$ equal to 54% and 37%, respectively. $var_{pcl}$ is 73%. The AP and IE constraint measurements are shown in Table 5.7.

Discussion

The kinematics optimized TKR design performs better (according to the defined objective functions) than the DePuy™ design. The optimum design is able to reach a greater flexion angle (+12.6%) before impingment between the femoral component and posterior edge of the UHMWPE insert occurs. $err_{tot}$ and $err_0$ are both smaller than the DePuy™ values (decreased by 53% and 130%, respectively). The overall AP
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Figure 5.12: Optimal TKR design in terms of kinematics. The design features a highly curved ML profile in the frontal plane. High conformity and curvature of the medial condyle in both planes produces a medial pivot type TKR design.

Table 5.6: Description of optimum TKR shape in terms of kinematics. Low radii of curvature in the frontal plane produces a highly curved ML profile. High conformity of the medial condyle is present in the frontal and sagittal planes.

<table>
<thead>
<tr>
<th></th>
<th>Medial</th>
<th>Lateral</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Femoral Component</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Frontal Radius</td>
<td>RFMed = 15.2 mm</td>
<td>RFLat = 24.3 mm</td>
</tr>
<tr>
<td>Condyle Spacing</td>
<td>WMed = 21.2 mm</td>
<td>WLat = 22.1 mm</td>
</tr>
<tr>
<td>Distal Sagittal Radius</td>
<td>RDMed = 25.0 mm</td>
<td>RDLat = 27.4 mm</td>
</tr>
<tr>
<td>Posterior Sagittal Radius</td>
<td>RPMed = 14.3 mm</td>
<td>RPLat = 15.9 mm</td>
</tr>
<tr>
<td><strong>UHMWPE Insert</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Frontal Radius</td>
<td>RFMed+CFMed = 15.2 mm</td>
<td>RFLat+CFLat = 24.3 mm</td>
</tr>
<tr>
<td>– unconformity</td>
<td>CFMed = 0 mm</td>
<td>CFLat = 0 mm</td>
</tr>
<tr>
<td>Sagittal Radius</td>
<td>RDMed+CSMed = 25.0 mm</td>
<td>RDLat+CSLat = 36.4 mm</td>
</tr>
<tr>
<td>– unconformity</td>
<td>CSMed = 0 mm</td>
<td>CSLat = 9.0 mm</td>
</tr>
<tr>
<td>Cup Length</td>
<td>LMed = 6.5 mm</td>
<td>LLat = 8.7 mm</td>
</tr>
</tbody>
</table>
Table 5.7: Overall AP and IE constraint at 0° and 30° for the kinematics optimized design. AP constraint is close to that of the natural knee, while IE constraint is lower. The collateral ligaments (not modelled) should contribute to IE constraint.

<table>
<thead>
<tr>
<th></th>
<th>Overall</th>
<th>About Neutral Point</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0° flexion</td>
<td>30° flexion</td>
</tr>
<tr>
<td>AP Constraint [N/mm]</td>
<td>37</td>
<td>20</td>
</tr>
<tr>
<td>IE Constraint [Nmm/deg]</td>
<td>246</td>
<td>139</td>
</tr>
</tbody>
</table>

constraint, as well as the AP constraint about the laxity neutral point are all closer to the physiological values reported in Table 5.3 than the DePuy™ design. The rotational constraint, however, is lower than the DePuy™ design which is already lower than the natural knee. While this might suggest that the kinematics optimized design lacks sufficient rotational constraint, it should be noted that the simulation does not include the MCL or LCL, both of which contribute towards rotational stability. The AP constraint is likely easier to match because the PCL, at least, is present in the model. The kinematics optimized design is slightly more sensitive to the presence of the PCL at 90° of flexion (\(\text{var}_{\text{pcl}} + 2\%\)) than the DePuy™ design.

It is important to note that the kinematics optimized design inherently makes some small consideration for wear performance. The constraints on maximum damage depths and fatigue damage scores were included during design optimization for kinematics. The reasoning behind this was that the design had to be feasible in terms of these constraints in order to act as an anchor point for multiobjective optimization. Another reason wear is inherently considered is in the size of the actual design space. The design space was reduced for simulation stability, mostly in terms of wear. This means a better design in terms of kinematics may have been excluded from the
optimization by shrinking the design space.

A weakness of the kinematics optimized design may exist in terms of stability. While the AP constraint is closer to that of the natural knee than the DePuy™ design, the constraint in TKR is a function of axial load. If less load is applied through the knee, the amount of constraint reduces linearly. This may lead towards instability in some scenarios.

5.5 TKR Multiobjective Optimization

5.5.1 Method

The weighted sum method was used for multiobjective design optimization considering UHMWPE wear and implant kinematics. The relative importance of the wear and kinematics objective functions was controlled by the weighting factor $w$ ($0 \leq w \leq 1$). Since the wear and kinematics objective functions from 5.4.3 and 5.4.4 were normalized, neither would dominate the weighted sum objective function (unless desired, in which case $w$ would be pushed towards 0 or 1). Any constraints which were applied during single objective wear or kinematics optimization were carried through to the multiobjective optimization. Thus, the mathematical problem statement for multiobjective design optimization considering wear and kinematics was:
Minimize $J_{MOO}(\bar{x}, w) = w[J_{wear}(\bar{x})] + (1 - w)[J_{kin}(\bar{x})]$

subject to:

\[ \begin{align*}
\delta_{max}(\bar{x}) & \leq 1 \text{ mm} \\
D_{max}(\bar{x}) & \leq 150 \\
\bar{x}_{min} & \leq \bar{x} \leq \bar{x}_{max} \\
0 & \leq w \leq 1
\end{align*} \]

where $\delta_{max}$ is the maximum damage depth and $D_{max}$ is the maximum damage score.

Figure 5.13 depicts the multiobjective optimization process for a single weighting function $w$. The time required for a single objective function evaluation was the sum of the time required for a wear and kinematics objective function evaluation, which was dominated by the computationally expensive wear simulations. Thousands of function evaluations were performed. In order to expedite the optimization process, many optimizations were run in parallel on a system capable of running up to 24 simultaneous optimization threads.

Multiobjective optimization was performed by considering different weighting functions and starting from different initial designs. Due to the presence of many local minima in the highly nonlinear objective function space, many optimizations ended at sub-optimal designs. The set of optimum designs were generated and plotted on a graph of $J_{wear}$ versus $J_{kin}$, in order to define a Pareto curve describing the relationship between wear and kinematics. Since separate wear and kinematics optimized designs had already been generated, the end-points of the curve were already defined, but
Figure 5.13: Flow chart depicting multiobjective optimization process for any given \( w \). \( w \) controls the relative importance of wear versus kinematics and is varied to produce different optimum designs.
the points in between were not. It was assumed that finding a point on the Pareto curve half-way between the wear and kinematics end-points could be achieved by using an initial design based on the weighted sum of the wear and kinematics optimum designs. This approach was used to define many initial designs at many initial weightings between wear and kinematics performance. Many random initial designs were also used, in order to expand the search for global optima.

5.5.2 Results

Anchor Points

The end points (anchor points) of the Pareto curve (see 2.8.3) were defined using the single objective wear and kinematics optimizations. The wear optimized design had to be assessed in terms of kinematics performance, and the kinematics optimized design had to be assessed in terms of wear performance.

The kinematics simulation with the wear optimized design predicted a maximum flexion angle \( \text{flex}_{max} \) of 128°, when impingement between the femur and posterior edge of the UHMWPE insert occurred. The overall laxity error compared to the natural knee \( \text{err}_{tot} \) was 67%. The laxity error about the neutral laxity point compared to the natural knee \( \text{err}_{0} \) was 85%. The importance of the PCL to knee laxity \( \text{var}_{pcl} \) was 72%.

The wear simulation with the kinematics optimized design predicted a volumetric wear \( W_{vol} \) of 25.7 mm\(^3\) per 3.5 million cycles, with a maximum damage depth \( \delta_{max} \) of 0.73 mm and a fatigue damage score \( D_{max} \) of 134. The resulting damage distribution is shown in Figure 5.14.
Figure 5.14: Resulting total damage distribution iso lines and contours (0.05 mm increments) for the kinematics optimized implant. Total damage includes both wear and creep contributions. The damage patches are more similar to those of the DePuy\textsuperscript{TM} design (Fig. 5.8) than the wear optimized design (Fig. 5.11).

Pareto Curve

The kinematics versus wear performance of each design evaluated during multiobjective design optimization is shown in Figure 5.15. Figure 5.16 highlights the set of optimum designs which define the Pareto curve. The resulting Pareto curve is shown in Figure 5.17. The Pareto curve was filtered from all of the available design performance data, such that each of the 20 points is a non-dominated optimum solution. While any point may outperform another in terms of one objective function, no Pareto point is outperformed in terms of both objective functions by any other single design. The curve depicts a competing relationship between wear and kinematics performance.

Since the kinematics performance measure was defined by several sub-measures,
Figure 5.15: The relative wear and kinematics performance of every design considered during multiobjective optimization. Points were obtained by saving objective function results during every function evaluation.

Figure 5.16: The relative wear and kinematics performance of every design considered, Pareto points highlighted. Pareto points were determined by using a filtering method, discluding any design which was outperformed by another design in terms of both objective functions simultaneously.
Figure 5.17: The relative wear and kinematics performance of the Pareto points defining the Pareto curve. Minimization of both $J_{\text{wear}}$ and $J_{\text{kin}}$ is desired. A distinct trade-off is present, requiring that wear performance must be sacrificed to improve kinematics, and vice-versa.

the performance of each with respect to $W_{\text{vol}}$ at each Pareto point was also investigated. Figure 5.18 shows $fle max$ versus $W_{\text{vol}}$ for each Pareto point. The correlation between the measures is also shown. $err_{tot}$, $err_0$, and $var_{pcl}$ versus $W_{\text{vol}}$ for each Pareto point are shown in Figures 5.19, 5.20, and 5.21, along with the correlation.

Secondary Performance Measures

Further investigation was performed in order to determine if any underlying relationships existed between the secondary performance measures (wear constraints), volumetric wear, and the maximum flexion angle. The relationship between $\delta_{\text{max}}$ and $W_{\text{vol}}$, and the relationship between $\delta_{\text{max}}$ and $fle max$, and the corresponding correlations are shown in Figures 5.22 and 5.23. The relationship between $D_{\text{max}}$ and $W_{\text{vol}}$, and the relationship between $D_{\text{max}}$ and $fle max$, and the corresponding correlations are shown in Figures 5.24 and 5.25.
Figure 5.18: Maximum flexion angle ($\text{flex}_{\text{max}}$) versus volumetric wear ($W_{\text{vol}}$) performance at each Pareto point and correlation. Minimization of $W_{\text{vol}}$ and maximization of $\text{flex}_{\text{max}}$ is desired. The data indicates a competing relationship between maximum flexion angle and volumetric wear.

Figure 5.19: Overall laxity error ($\text{err}_{\text{tot}}$) versus volumetric wear ($W_{\text{vol}}$) performance at each Pareto point and correlation. Minimization of both $W_{\text{vol}}$ and $\text{err}_{\text{tot}}$ is desired. The data indicates a competing relationship between overall laxity error and volumetric wear.
Figure 5.20: Neutral point laxity error ($err_0$) versus volumetric wear ($W_{vol}$) performance at each Pareto point and correlation. Minimization of both $W_{vol}$ and $err_0$ is desired. The data indicates a competing relationship between neutral point laxity error and volumetric wear.

Figure 5.21: Importance of PCL ($var_{pcl}$) versus volumetric wear ($W_{vol}$) performance at each Pareto point and correlation. Minimization of both $W_{vol}$ and $var_{pcl}$ is desired. The data does not indicate any clear relationship between the importance of the PCL and volumetric wear.
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Figure 5.22: Maximum damage depth ($\delta_{\text{max}}$) versus volumetric wear ($W_{\text{vol}}$) performance at each Pareto point and correlation. Minimization of both $\delta_{\text{max}}$ and $W_{\text{vol}}$ is desired. The data suggests a weak relationship between maximum damage depth and volumetric wear.

Figure 5.23: Maximum flexion angle ($f\text{l}_{\text{max}}$) versus maximum damage depth ($\delta_{\text{max}}$) at each Pareto point and correlation. Minimization of $\delta_{\text{max}}$ and maximization of $f\text{l}_{\text{max}}$ is desired. The data suggests a weak relationship between maximum flexion angle and maximum damage depth.
Figure 5.24: Fatigue damage score ($D_{\text{max}}$) versus volumetric wear ($W_{\text{vol}}$) performance at each Pareto point and correlation. Minimization of both $D_{\text{max}}$ and $W_{\text{vol}}$ is desired. The data suggests a strong relationship between fatigue damage score and volumetric wear.

Figure 5.25: Maximum flexion angle ($\text{flex}_{\text{max}}$) versus fatigue damage score ($D_{\text{max}}$) at each Pareto point and correlation. Minimization of $D_{\text{max}}$ and maximization of $\text{flex}_{\text{max}}$ is desired. The data suggests a weak relationship between maximum flexion angle and fatigue damage score.
The relationship between laxity and flexion kinematics performance was also studied. The relationships between \( err_{tot} \) and \( flex_{max} \), \( err_0 \) and \( flex_{max} \), and \( var_{pcl} \) and \( flex_{max} \), along with corresponding correlations, are shown in Figures 5.26, 5.27, and 5.28.

![Figure 5.26: Overall laxity error (\( err_{tot} \)) versus maximum flexion angle (\( flex_{max} \)) at each Pareto point and correlation. Minimization of \( err_{tot} \) and maximization of \( flex_{max} \) is desired. The data does not indicate any relationship between overall laxity error and maximum flexion angle.](image)

5.5.3 Discussion

**Anchor Points**

In terms of \( flex_{max} \) and \( var_{pcl} \), the wear optimized design performed on par with the DePuy\textsuperscript{TM} TKR design, and actually performed better in terms of \( err_{tot} \) and \( err_0 \). Considering the history of clinical success of the DePuy\textsuperscript{TM} design, the results suggest that the wear optimized design should still perform sufficiently in terms of kinematics.

The kinematics optimized design performed much worse in terms of wear when
Figure 5.27: Neutral point laxity error \( (\text{err}_0) \) versus maximum flexion angle \( (\text{flex}_{\text{max}}) \) at each Pareto point and correlation. Minimization of \( \text{err}_0 \) and maximization of \( \text{flex}_{\text{max}} \) is desired. The data indicates a weak relationship between neutral point laxity error and maximum flexion angle.

Figure 5.28: Importance of PCL \( (\text{var}_{\text{pcl}}) \) versus maximum flexion angle \( (\text{flex}_{\text{max}}) \) at each Pareto point and correlation. Minimization of \( \text{var}_{\text{pcl}} \) and maximization of \( \text{flex}_{\text{max}} \) is desired. The data does not indicate a relationship between the importance of the PCL and maximum flexion angle.
compared to the DePuy$^\text{TM}$ design. $W_{\text{vol}}$ was 52.8% higher than the DePuy$^\text{TM}$ design, and $\delta_{\text{max}}$ and $D_{\text{max}}$ were also much higher. The increased maximum damage depth can be attributed to the increased thickness of the UHMWPE insert. The increased damage score is likely caused by the large / flat sagittal plane geometry of the UHMWPE insert. This would likely cause increased AP displacement of the femorotibial contact location, increasing the likelihood for fatigue damage. This profile, however, also contributes to the femoral rollback required for achieving deeper flexion.

The difference between the wear and kinematics designs is most evident when looking at the frontal plane geometry. The radii of curvature in the frontal plane are much higher for the wear optimized design versus the kinematics optimized design. The large frontal radii of curvature in the wear optimized design would increase the contact area between the two components and reduce the contact stresses, which contributed to the lower wear rates. In the sagittal plane, the wear optimized design again has larger radii of curvature than the kinematics optimized design. The smaller radii of curvature in the sagittal plane provided a long flat area on the contact surface of the UHMWPE insert to allow greater femoral rollback, and higher flexion. The wear optimized design again increased contact area and reduced contact stresses. Having less mobile femorotibial contact locations helped to reduce the fatigue damage score in the wear optimized design.

**Pareto Curve**

The Pareto curve shows that there is a clear trade-off between wear and kinematics performance (Fig. 5.17). When a high importance is placed on wear performance,
the objective function can be reduced significantly, however this comes at a great price in terms of kinematics performance once the wear objective function needs to drop below approximately 0.2. The points do not form a smooth curve, but a noisy or stepped curve. This is likely due to the presence of many local minima, as well as some noise in the objective functions themselves. The wear objective function is known to contain a small amount of random noise that can affect the Pareto curve, and was also a problem affecting the finite differencing stage during optimization.

The kinematics objective function is the sum of unconstrained flexion kinematics and implant laxity performance, so the individual performances were compared with the volumetric wear performance for each Pareto point. In terms of maximum flexion angle (Fig. 5.18), aside from 2 outlier points, there appears to be a correlation \( r^2 = 0.62 \) between maximum flexion angle and volumetric wear production. This suggests that there is almost a linear trade-off between maximum flexion angle and volumetric wear production for optimum designs. This relationship could be linked to the different sagittal radii of curvature between wear and kinematics optimized designs. Smaller radii of curvature in the kinematics-optimized design improves femoral rollback. The smaller radii of curvature, however, would increase contact pressures, and could lead to increased volumetric wear.

While \( \text{err}_{\text{tot}} \) and \( \text{var}_{\text{pcl}} \) show only weak correlations with \( W_{\text{vol}} \), there is a stronger correlation between neutral point laxity \( (\text{err}_0) \) and \( W_{\text{vol}} \) \( (r^2 = 78) \). The curve (Fig. 5.20) strongly indicates that there is a competing relationship between obtaining natural knee laxity characteristics (about the laxity neutral point) and volumetric wear production. The natural knee provides little constraint against small displacements or rotations. This characteristic is often not reproduced by TKR, because the shape of
TKR provides high constraint under axial loads. In the kinematics-optimized design, however, a flat AP profile in the sagittal plane provides little constraint about the laxity neutral point. This reduced constraint, however, increased the amount of AP displacements during wear simulation, leading to increased volumetric wear.

**Secondary Performance Measures**

There were weak correlations between the maximum damage depth ($\delta_{max}$) and volumetric wear / maximum flexion angle. $\delta_{max}$ was dominated by creep damage, so it is likely that the thickness of the UHMWPE beneath the contact surface played the largest role in the maximum damage depth. The maximum damage depth, however, did seem to increase with the amount of volumetric wear as well as the maximum flexion angle.

There is a strong correlation ($r^2=80$) between the damage score and the amount of volumetric wear (Fig. 5.24). This suggests that designs which exhibit increased volumetric wear may also be more likely to experience fatigue damage such as pitting or delamination. TKR designs optimized for reduced abrasive / adhesive wear may inadvertently be optimized for reduced likelihood of fatigue damage as well. The relationship between fatigue damage and maximum flexion angle also shows a weak correlation (Fig. 5.25), where increased flexion is accompanied by increased fatigue damage scores.

There is not a very strong correlation between any laxity measure and the maximum allowable flexion angle. The strongest correlation in this group is the relationship between $err_0$ and $flex_{max}$ (Fig. 5.27). Designs with better neutral point laxity scores can also exhibit a high range of motion.
Chapter 6

Summary and Conclusions

6.1 Summary

The global objective of this work was to perform multiobjective design optimization of a total knee replacement considering wear and kinematics. A set of necessary sub-objectives were outlined in 1.3, each of which had to be completed in order to meet the defined global objective.

Sub-objective 1: Wear Testing and Simulation

The first sub-objective was the development and validation of a numerical framework for wear simulation. The FE solver ANSYS\textsuperscript{TM} was used to perform contact analysis and calculate contact stress and sliding conditions during simulated wear testing of TKR components. A novel frictional-work based wear model was formulated based on previous models described in the literature and tuned through in-house experimental work. The wear model was validated using further experiments under different applied kinematics. The use of a different set of input waveforms was novel to this work,
and no other TKR wear models have been so thoroughly validated. This work also represents the most advanced TKR wear simulations to date, combining a frictional-work based wear model which accommodates for strain hardening, an UHMWPE creep model, and a fatigue-based UHMWPE damage model. The validated wear simulation framework provides a means of comparing different TKR designs in terms of wear performance during design optimization.

**Sub-objective 2: Kinematics Testing and Simulation**

The second sub-objective was the development and validation of a numerical framework for kinematics simulation. The rigid body dynamics solver MSC.Adams™ was used to perform simulated laxity and unconstrained flexion simulations on TKR components. Several simulation parameters were tuned using optimization to maximize the agreement with experimental results. One especially important tuning parameter was compliance of the testing apparatus, which had to be included in the simulation in order to match experimental results. Experiments also found that the laxity and flexion characteristics of an implant-grade metal-on-polyethylene TKR can be reasonably approximated using ABS plastic prototypes. The most significant differences between CoCr-UHMWPE versus ABS plastic components are the coefficients of friction and the tendency for ABS plastic components to stick during changes in counterface direction (stiction). Simulations had difficulty matching this sticking behavior. Good agreement between several random ABS plastic TKR designs simulated experimentally and numerically provided validation of the numerical model. The validated kinematics framework forms a basis for more advanced kinematics simulations necessary for benchmarking different TKR designs during design optimization.
**Sub-objective 3: Parametric Modelling of TKR**

A parametric modeller to generate TKR FE and STL CAD models was the third sub-objective of this work. In order to perform wear and kinematics simulations, designs had to be represented by computational models. To perform design optimization, these models needed to be able to change shape as demanded by the optimization algorithm. It was also necessary that the two different model types, FE and STL CAD, were identical shapes in order to provide accurate performance evaluations in terms of wear and kinematics. This was addressed by building both models within the FE pre-processor HyperMesh™, which built the models based on instructions provided as TCL/TK commands. A total of 14 design variables controlled the shape of the parametric TKR femoral component and UHMWPE insert. The number of design variables and the range of these design variables were determined after hundreds of simulations, considering the robustness of the parametric modeller, the robustness of the simulation routines, and the impact on implant performance. No such parametric TKR model has ever been reported in the literature, and this is the first model which is suitable for use during three-dimensional design optimization.

**Sub-objective 4: Separate Single Objective Optimizations**

The fourth sub-objective was to perform single objective design optimization, considering wear and kinematics separately. Single objective optimization considering wear was performed using the validated wear simulation framework. The predicted volumetric wear of the optimized design was 56.8% lower than the wear of a commercially available TKR design under matching simulation conditions. The maximum damage depth and damage score increased (20.8% and 33.3%, respectively) - but this was due
to a thicker UHMWPE insert and greater anterior-posterior counterface motion. The thickness of the UHMWPE insert was not an active design variable during optimization, and is assumed to vary from patient to patient. The greater anterior-posterior counterface motion was the result of reduced sagittal plane conformity (which helped reduce volumetric wear by reducing contact area). The design optimized for wear without any consideration for kinematics still performed adequately in terms of kinematics when compared to the DePuy™ design, achieving a range of motion and laxity measures similar to the clinically successful design.

Single objective optimization considering kinematics was performed using the validated kinematics simulation framework. The simulations were modified slightly – by the addition of springs to represent the contribution of the posterior cruciate ligament. Design optimality was a function of the maximum allowable flexion range of motion, the likeness to natural knee laxity characteristics taken from the literature, and reduction of the laxity sensitivity to the PCL. Compared to a commercially available TKR design, the flexion range of motion was increased by 12.6%. The laxity characteristics of the TKR were much closer to those of the natural knee, however the design was slightly more sensitive to the PCL.

Sub-objective 5: Multiobjective Optimization

The final objective was to perform multiobjective design optimization considering wear and kinematics performance. This was achieved by combining both validated numerical frameworks and using the weighted sum approach. An objective function was minimized which represented the weighted sum of the wear and kinematics performance, with relative importance of either measure controlled by a weighting factor.
By varying the weighting factor and obtaining a set of optimum designs, a Pareto curve was defined – a curve which graphically depicts the best trade-off between wear and kinematics performance. The end points of this curve were the wear and kinematics optimized designs from sub-objective 4. This allowed a reduction of the search scope for optimum designs, by only considering designs between these two optimums as start points for multiobjective optimization. This was done by interpolating between the wear and kinematics optimized design vectors based on the desired relative importance. The curve shows that there is, in fact, a competing relationship between wear and kinematics. A study of individual performance measures showed that there were strong trade-offs between maximum flexion angle and volumetric wear, and neutral point laxity and volumetric wear. The greater contribution of this information is that designers can choose which performance measure to favour while knowing exactly how much performance must be sacrificed in terms of the other measure, while still maintaining an optimum design.

6.1.1 Limitations to Address in Future Work

Statistical Significance during Wear Experiments

Quite a few factors made it necessary to reduce the scope of the experiments. The biggest factor was cost, as commercially available implant components are expensive. It was not feasible to purchase a large number of samples, as well as the associated supplies which are consumed during experiments (such as bovine serum). Time was also a limiting factor. Having access to only a single-station knee simulator, experiments had to be performed one after another, and each wear experiment took approximately 2 months to complete. Apparatus failures were a frequent issue. The
For 5\textsuperscript{TM} testing machine broke down several times over the course of the experiments, which delayed testing further.

Despite the limited amount of experimental data, clear trends were apparent in the results. Regarding the dramatic increase in volumetric wear accompanying increased IE rotation, these trends are in agreement with statistically significant results observed in the literature [21–29]. Future work, however, should address this by performing further experiments with commercially available implant components. Once agreement with the numerical model can be maintained with statistically significant sample sizes, a much stronger case for model validity would be supported.

**Creep and Fatigue Damage Model Validation**

Attempts were made to validate the creep model used in the wear simulation, as it has not previously been applied to a TKR damage model. The creep damage at the contact surface of an axially loaded UHMWPE insert sample was measured using the laser scanner. Unfortunately, the damage depths reported by the laser scanner are questionable, and provided more of a qualitative depiction of the damage depth distribution. Attempts were made to better quantify the damage depths using a coordinate measuring machine (CMM), but the accuracy of this equipment was also questionable due to its age and the lack of a documented calibration history. No attempt was made to validate the fatigue damage model which was adopted in this work. The purpose of including this model was only to provide a comparison between different designs in terms of the likelihood for fatigue damage, not an exact quantitative measure. The value was used as a constraint during optimization simply to steer the optimizer away from designs which may be more likely to exhibit fatigue.
Future work should address creep model validation by performing creep-only (axial load only) experiments with implant components. Surface damage measurements made with a higher accuracy laser scanner or an automated CMM machine would be necessary. The fatigue damage model could be validated by long-term wear experiments. The 3.5 million cycle termination point for the wear experiments may not have been long enough for any fatigue damage to occur. Higher cycle counts or artificial aging processes (such as oxidation) may permit more fatigue damage and allow for model validation [100, 114].

**Contribution of Fluid-Film Lubrication and Heating**

The UHMWPE wear model made no attempt to account for the contributions of fluid-film lubrication effects at the contact surface of the UHMWPE insert. Previous experimental work using implant grade materials in a tribotester has shown that fluid-film lubrication may play a role in TKR wear [115]. Modelling the fluid dynamics at the contact surface between the femoral component and UHMWPE insert would be extremely complex. Including this with the FE contact analysis would have been exceedingly difficult, especially for a model designed to be used in the iterative process of design optimization. Frictional heating and the effects on UHMWPE compliance was also neglected. The stiffness properties and yielding behaviour of UHMWPE are sensitive to temperature, which could increase at the contact surface as a result of frictional work. Again, modelling such a phenomenon would greatly increase the complexity of the simulation. Considering the strong agreement between experiment and simulation results with the tuned model, it may be possible that these effects are
negligible for the DePuy\textsuperscript{TM} implant components used in this study.

**ABS Plastic Components for Kinematics Validation**

The kinematics simulations were validated by comparison to experimental results using ABS plastic prototypes. Although the results showed that ABS plastic components provided a good approximation of implant kinematics with implant-grade materials, this agreement under different contact conditions and different levels of component conformity may not be maintained. The stiction behavior of the ABS component implants, for example, was always present to some extent, while rarely observed when using an actual commercially available implant.

Future work could focus on validating the kinematics simulation against experimental results with a number of different implants made from implant-grade materials. These could be existing commercially available components, or unique prototypes which could have more varied geometries. The drawback of using commercially available components is the similarity between the shapes of most implant designs, which would only validate a small portion of the design space. The drawback of unique prototypes is the cost to have them manufactured.

**Parametric Model and Design Space**

The original intent of this work was to make the parametric model as robust as possible, allowing a very large design space for the optimizer to search. A myriad of different TKR design forms exist outside of the classic condylar design modelled in this study [116]. The resulting design space, however, had to be reduced significantly. This was largely due to problems with the parametric modeller, where conflict between
design elements and meshing failures forced several design variables to be set to constant values. Simulation failures also required further reduction of the design space. While the optimizer was modified to be able to manage simulation failures, it was preferred to reduce the design space and the likelihood of failures. Computational efficiency was a further driving force in design space reduction. The length of time required for optimization grows with the number of design variables.

Future work should look at different optimization methods to allow for a larger design space. Using an optimizer which does not rely on gradient information, for example, would allow for discrete design variables which would greatly increase the design space (for example, allowing the presence of a cam mechanism, like those of cruciate substituting designs, to be turned on or off). More powerful computational resources will also make larger studies on implant shape more feasible.

**Kinematics Objective Function Definition**

"Optimal" kinematics was very difficult to define. While one desires to make the artificial knee function the same as a natural knee, there are too many different aspects of natural knee performance to consider simultaneously (walking, jogging, running, stair climbing, squatting, cutting motions, etc.). The objective function had to be limited to something that could be simulated, with confidence in the simulation results. Unconstrained flexion was chosen based on the assumption that a knee which promotes natural flexion kinematics is likely to promote natural kinematics under other motions. Laxity was chosen because of the suspected relationships with flexion and wear performance [8]. While addressing flexion and wear, there was a strong likelihood of designing a knee which had infeasible laxity characteristics. With the
recent development of TKR laxity testing standards [89], the development of the simulation was not difficult, nor was the validation, so the inclusion of laxity was deemed appropriate.

Including the PCL for some simulations in order to observe the impact on knee kinematics was an aspect of the simulation which could not be validated. While the PCL stiffness properties and insertion points were taken from the literature [74, 81, 83, 110], the PCL model is known to be rather simplified. Regardless, it was important to somehow address the contribution of such an important part of knee anatomy. Further justification for the lack of validation is that the objective function sought to minimize the impact of the PCL ($var_{pcl}$). This means that for the optimum designs that were developed, the importance of the PCL modelling technique is minimized by minimizing the overall PCL contribution. This was not the reason why PCL contribution was minimized, however. As stated earlier in the thesis, PCL function was actually minimized in order to allow TKR success to be less sensitive to ligament balancing. It is important to note, however, that the value for $var_{pcl}$ did not change very much during optimization, and still contributed largely to knee constraint characteristics at 90° of flexion.

Another weakness is the lack of any account for ligament wrapping. While the natural PCL may have to wrap around some anatomy between the origin and insertion points, the simulated PCL will always maintain a straight line. This means that the simulated PCL may be under less strain than would be in reality.

Future work should focus on developing a stronger simulation framework for both laxity and unconstrained flexion. This will require greater computational resources and validation, likely requiring natural knee specimens for testing. The definition of
the kinematics objective function could also be addressed. While the objective function could be expanded to include more performance measures, this poses a problem in terms of weighting. The relative importance of different performance measures must be defined, as was done in this thesis, and this becomes more difficult as more performance measures are added. The nonlinearity of the design space is also likely to increase, greatly increasing the optimization time. Multiobjective optimization considering several kinematics-related performance measures may also be of interest.

**Stability**

As discussed earlier, the stability of a natural knee is provided by a combination of contact geometry and soft tissue contributions, while the stability of the replaced knee is more sensitive to the contact geometry and the axial load [71]. The constraint of the candidate TKR designs considered in this work was always calculated under 710 N of axial load (1X body weight of a 72 kg /160 lbs individual), taken from the proposed ASTM standard [89]. Depending on the situation, the actual load for through the knee will vary greatly (much higher during the stance phase of gait, but possibly lower during static standing poses, depending on muscle contributions). The drawback of this assumption is that the artificial knee may not provide sufficient constraint when less axial load is provided.

Future work should investigate the importance of stability and the affect on a kinematics optimized design. It is conceivable that a trade-off between flexion and stability exists, but could be addressed by a design capable of achieving different levels of constraint at different flexion angles.
Local Minima in Design Optimization

While a great amount of computational effort was used in order to search the design space as thoroughly as possible, it is still possible that the optimum designs found are not the true global optima within the design space. The design space proved to be extremely nonlinear, meaning that very many local minima existed and multiple initial designs were used as optimization start-points in order to maximize the likelihood of finding the true global optima.

The only possible way of knowing that the optimum designs are in fact global optima would be to rigorously search the entire design space. At this time, such an approach is infeasible. Considering the fact that the parametric model is defined by 14 design variables, if one were to evaluate the TKR performance of every possible combination of design variables set to their maximum and minimum values, it would require 16,384 function evaluations (and each function evaluation takes approximately 5 hours). If one considers the fact that the relationship between a design variable and an objective function is often nonlinear, considering only the maximum and minimum value is insufficient, and the actual computational effort needed to sufficiently search the entire design domain increases dramatically. Faced with such a large design space, it is impossible at this time to say the global optima have definitely been found. For future work, as computational resources continue to advance, it may be possible to examine the entire design space.
6.2 Conclusion

In conclusion, a trade-off between wear and kinematics performance was identified and described using a Pareto curve, supporting the hypothesis based on the findings of Sathasivam and Walker [8]. These results could not have been obtained without the numerical frameworks for wear and kinematics simulation which were developed and validated, as well as the parametric modelling and multiobjective optimization frameworks which were used.

Using the Pareto curve, a designer can input their own preference for wear or kinematics while knowing how much they must sacrifice in terms of the other performance measure. Due to the shape of the curve, however, one may find that the best trade-off between these competing performance measures can be achieved using a weighting factor ($w$) around 0.5 – placing equal importance on wear and kinematics. The sacrifice required of one design variable for only marginal improvements in the other increases greatly with $w$ values further away from 0.5.

One must also consider that while impressive results have been achieved using design optimization, clinical results are going to be a function of many more factors. The preoperative range of motion, surgical technique, rehabilitation, disease progression before knee replacement and activity level will all factor very largely into the postoperative success of a total knee replacement [64, 66, 67].

The future vision for the application of multiobjective optimization to TKR is in patient-specific design, and depends on advances in imaging techniques, clinical biomechanics and gait lab capabilities, material breakthroughs, and rapid prototyping technology. In the future, a patient-specific Pareto curve could be generated for every candidate for a TKR, allowing the health care provider to determine the most
appropriate balance between wear and kinematics, and TKR shape, for that situation. A custom implant would then be manufactured using rapid prototyping techniques. In the meantime, health care providers can use the developed Pareto curve to aid in the selection of the most appropriate TKR design for their patient from the spectrum of commercially available designs.
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Appendix A

Cleaning Samples

The method of cleaning the UHMWPE samples before gravimetric measurements was adapted from ASTM F-1714 [103], a guide for gravimetric wear assessment of artificial hips and ISO 14243-2 [41], methods of measurement of TKR wear. Due to unavailability of certain materials and resources, the cleaning procedure here deviates from the standard, but results indicate that the simplifications do not significantly effect the experiment outcome.

1. Gently wipe samples with clean paper towel to remove serum particles - sample should appear clean.

2. Rinse well with deionized water.

3. Clean in an ultrasonic bath.

   5 min. in deionized water.

   Rinse well with deionized water.
10 min. in 10 mL of liquid ultrasonic cleaning detergent plus 500 mL of deionized water.

Rinse well with deionized water.

10 min. in deionized water.

Rinse well with deionized water.

3 min. in deionized water.

Rinse well with deionized water.

4. Dry with air blower until no water is visible on component.

5. Soak in 95% methyl alcohol for 5 min.

6. Dry with air blower for 10 min., alternating sides.

7. Dry in a vacuum jar at -690 mm Hg for 30 min.

After removing from the vacuum jar, the sample should acclimatize in the same room as the analytical balance for 30 minutes before any measurements are made. The components should not be handled manually but with Kelly forceps once dry.
Appendix B

Kinematics Results Plots
Figure B.1: The untuned simulation results using the DePuy\textsuperscript{TM}-STL model (blue) compared to experiments using DePuy\textsuperscript{TM}-ABS DePuy\textsuperscript{TM} components (red). Unconstrained flexion kinematics results are shown at the top, with laxity results below.
Figure B.2: The tuned simulation results using the DePuy\textsuperscript{TM}-STL model (blue) compared to experiments using DePuy\textsuperscript{TM}-ABS DePuy\textsuperscript{TM} components (red). Unconstrained flexion kinematics results are shown at the top, with laxity results below.
Figure B.3: Simulation results using the Design-A-STL model (blue) compared to experiments using Design-A-ABS components (red). Unconstrained flexion kinematics results are shown at the top, with laxity results below.
Figure B.4: Simulation results using the Design-B-STL model (blue) compared to experiments using Design-B-ABS components (red). Unconstrained flexion kinematics results are shown at the top, with laxity results below.
Figure B.5: Simulation results using the Design-C-STL model (blue) compared to experiments using Design-C-ABS components (red). Unconstrained flexion kinematics results are shown at the top, with laxity results below.
Appendix C

Computational Framework

The computational framework is described graphically. Figure C.1 depicts the overall computational framework which ties together the individual wear and kinematics simulations for optimization. Figure C.2 depicts the computational framework for the parametric modeller. The framework is supplied with the design vector and mesh parameters, along with some program settings. Figure C.3 depicts the computational framework for unconstrained flexion simulations. This program relies on the presence of a STL CAD model of the implant components. The program returns the flexion characteristics and PCL contributions. Figure C.4 depicts the computational framework for laxity simulations. This program also relies on the presence of a STL CAD model of the implant components, returning the laxity characteristics and PCL contributions. Finally, in Figure C.5, the computational framework for wear simulation is outlined. This framework requires that a FE model of the implant components already exists. The program returns the volumetric wear, maximum damage depth and damage score after 3.5 million cycles.
Figure C.1: The overall computational framework.

- **run_opt**: defines simulation parameters and initiates fmincon for optimization.
- **fmincon**: performs optimization from initial design, will call on results_analysis for function evaluations.
- **run_analysis**: checks results_log.txt for pre-existing results, otherwise performs the required analysis.
- **build_model**: builds the FE and STL CAD models.
- **get_fitness_flex**: performs unconstrained flexion simulation with and without PCL contributions.
- **get_fitness_lax**: performs AP and IE laxity simulation at 0 and 30 degrees, then at 90 degrees with and without PCL contributions.
- **wear_sim**: performs wear simulation using frictional work based model, creep, and fatigue damage score.
- **cleanup**: deletes the FE and STL CAD models simulations delete there own working files.
Figure C.2: Detailed illustration of the parametric modeller computational framework.
Figure C.3: Detailed illustration of the unconstrained flexion kinematics computational framework.
Figure C.4: Detailed illustration of the laxity simulation computational framework.
Figure C.5: Detailed illustration of the wear simulation computational framework.