

**OPTIMIZATION OF DYNAMIC SIMULATIONS TO
IDENTIFY MOVEMENT PATTERNS THAT
SIMULTANEOUSLY REDUCE THE RISK OF
INJURY AND ENHANCE HUMAN PERFORMANCE**

A Dissertation Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville

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May 2021

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DEDICATION

To my mother, Anupama Gupta, for always believing in me

And

To the sport of volleyball that taught me valuable life lessons and gave me a
direction in my youth

ACKNOWLEDGEMENTS

I want to thank my advisor, Dr. Jeffrey Reinbolt, for his guidance throughout my PhD journey. His critical thinking, problem solving, and ethical research principles make him an ideal mentor. I liken his mentoring style to a rudder on a boat. He made sure that my PhD boat moved in the right direction while I could still be the engine doing all the hard work and learning the best lessons in the process.

I want to thank Dr. Cyril Jon Donnelly for giving me the opportunity to visit his labs and allowing me to be a part of his research. His critical thinking and ability to integrate a variety of research areas to enhance the applicability of our research has been an inspiring lesson.

I would also like to thank members of my dissertation committee, Dr. Cyril J Donnelly, Dr. Dustin Crouch, and Dr. Zhenbo Wang for their time and advice. They challenged me to produce the best quality research through constructive criticism on both research and writing.

I want to thank Dr. Cyril Donnelly and Dr. Jody Jensen for allowing me to use data collected in their laboratories for my research. This data was invaluable and critical to my research.

I also want to thank my partner, Nancy Nguyen, for patiently supporting me throughout my PhD journey. Her patience, love, and support always kept my spirits high and allowed me to do my best work.

ABSTRACT

Every movement, whether routine or sporting, achieves certain goals. Routine movements like walking takes us from one place to the other and sporting movements like hitting a volleyball help win the game. But each motion puts strain on certain joints of the body putting them at risk of injury. Walking can lead to chronic disorders like knee osteoarthritis over the years. Hitting a volleyball can put the shoulder at risk of a rotator cuff injury. The purpose of this work is to find optimal movement patterns that enhance human ability to achieve the goals of the movement, but at the same time, reduce the risk of injury while performing the movement.

Musculoskeletal modeling and simulation are powerful tools that allow researchers to generate dynamic simulations of human movement and answer questions like “what is the effect on certain biomechanical parameters if the movement changes in certain ways?” Additionally, the simulation environment can be combined with optimization methods to essentially check thousands of variations of the same overall movement and find the optimal one that both enhances human ability and reduces the risk of injury, something that cannot be achieved in experimental studies.

In this work, we used optimization methods combined with musculoskeletal modeling and simulations to find optimal whole-body, participant-specific movement patterns for landing, volleyball hitting, and walking that reduce the risk of anterior cruciate ligament injury, enhance hitting performance while reducing the

risk of shoulder injury, and reduce the risk of progression of knee osteoarthritis, respectively. While doing so, a) guidelines were established that help the research community distinguish accurate simulations of dynamic simulations from errored ones, b) concepts from other disciplines like robotics were integrated to human simulation platforms to enhance dynamic consistency of human simulations, and c) the computational speed of the optimization process was reduced from days to minutes, making the process clinically relevant. Additional care was taken to ensure that the optimal whole-body movement patterns are participant-specific and not too different from the experimental data, ensuring that these new patterns can potentially be learned, enhancing the practical applicability of this work.

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Filename: Supplementary_Data_2_1A.avi

Format: Video file (.avi format)

Supplementary data 2.1.B. Dynamic nature of the new guidelines and their comparison to the original 2015 recommendations for gait.

Filename: Supplementary_Data_2_1B.avi

Format: Video file (.avi format)

Supplementary data 2.2.A. MATLAB results of zero moment point computations and when each of the three guidelines are violated during single-leg jump-landing.

Filename: Supplementary_Data_2_2A.avi

Format: Video file (.avi format)

Supplementary data 2.2.B. MATLAB results of zero moment point computations and when each of the three guidelines are violated during gait.

Filename: Supplementary_Data_2_2B.avi

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Filename: Supplementary_Data_2_3A.avi

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Filename: Supplementary_Data_2_3B.avi

Format: Video file (.avi format)

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Filename: checkGuidelines.m

Format: MATLAB code (.m format)

Supplementary data 4.1. Representation of the primary mechanism to enhance performance without increasing the risk of shoulder injury during power phase.

Filename: Supplementary_Data_4_1.mp4

Format: Video file (.mp4 format)

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Supplementary data 6.1. Frontal plane view of pre- and post-optimization kinematics during stance phase of the affected leg from one trial from each of the four participants.

Filename: Supplementary_Data_6_1.mp4

Format: Video file (.mp4 format)

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CHAPTER ONE

INTRODUCTION

1.1. Project summary

While all movements achieve certain goals, at the same time, they also strain certain joints of the body, putting them at a risk of injury. Routine movements like walking help us get from one place to the other, but while doing so can cause degenerative disorders over the years such as knee osteoarthritis (Fregly et al., 2012). Similarly, quick movements like hitting a volleyball high and fast are important to score points and win the game, but can put the shoulder at risk of a rotator cuff injury (Briner and Kacmar, 1997). Therefore, it is necessary to find optimal movement patterns that would allow, or even enhance, the human ability to perform the goals of the movement, but at the same time, not predispose people to risk of injury.

Musculoskeletal modeling and simulations have been used to represent human movement in a computer environment and ask “what if” questions. These dynamic simulations of human movement allow researchers to study the relationship between certain biomechanical parameters in a controlled environment, that is, the effect of changing one parameter can be studied while keeping all other parameters constant. This is very hard to achieve experimentally.

Optimization methods can be combined with musculoskeletal modeling and simulations to essentially study thousands of variations of the same general movement and choose the optimal one that enhances human performance while reducing the risk of injury.

In this work, we used optimization methods combined with musculoskeletal modeling and simulations to find optimal whole-body, participant-specific movement patterns for three different movements. We refer to the method of combining optimization methods with musculoskeletal modeling and simulations to find optimal movement patterns as an optimal dynamic simulation generation (ODSG) process. The three movements studied and their particular goals are: First, single-leg jump-landing task to reduce the risk of anterior cruciate ligament (ACL) injury. Second, volleyball hitting/spiking task to enhance performance parameters and at the same time reduce the risk of shoulder injury. Third, walking gait to reduce the progression of knee osteoarthritis.

While using the ODSG process to find optimal movement patterns, we also enhanced the involved dynamic simulation and optimization methods. First, we established guidelines that help researchers distinguish the dynamic simulations that accurately represent the movement in computer environment from the errored ones. Second, we integrated concepts from robotics to the computational musculoskeletal modeling process to make it more robust and enhance the dynamic consistency of simulations. Third, we reduced the computational time of the ODSG process from days to minutes to make it clinically relevant.

To enhance practical applicability of our simulation studies, we ensured that the optimal movement patterns generated through simulations were participant-specific and close to the experimental data. This ensures that these new movement patterns can potentially be learned by the individuals.

1.2. Research significance

This research is significant in multiple ways. First, the optimal movement patterns found in this work can potentially address critical biomechanical needs associated with the respective movement and help establish new biomechanically informed training protocols. Single-leg jump-landing is known to increase the risk of ACL injury (Hewett et al., 2006) and the optimal movements found in our work can help athletes understand how to perform safer landings. Similarly, walking gait can increase the progression of the degenerative disorder knee osteoarthritis (Fregly et al., 2012) in some people over the years, and the optimal gait patterns we found in this work can help mitigate this progression. Additionally, this work also establishes methods that can be used to achieve a performance-injury prevention balance. Performance and injury prevention are two important pillars of long-term success in sports, and they are often seen as mutually exclusive. It is generally perceived that too much focus on performance can increase the risk of injury, while too much focus on injury prevention might hinder performance. Our work finds optimal movement patterns for volleyball hitting that increase the performance parameters while simultaneously reducing the risk of injury. This finding is significant as it proves that performance and injury prevention are not always mutually exclusive and also establishes methods that can be used to achieve both goals simultaneously.

Our work is also significant on the methodology front. We established new guidelines that help researchers distinguish dynamically consistent simulations

from errored ones. These guidelines can have major implications since we found that the existing recommendations on the allowable simulations (Hicks et al., 2015) can potentially accept dynamically inconsistent simulations, which can subsequently affect the results and clinical interpretations of simulation studies.

The ODSG process is currently far from clinically relevant because of multiple limitations (Donnelly et al., 2012c). In this work, we enhanced the robustness of the ODSG process in multiple ways to the extent that it can now be considered a clinically viable tool. First, we increased the dynamic consistency between a simulation's external forces and inertial forces by integrating concepts from robotics. Second, we adapted the ODSG process to concurrently handle both performance goals and injury prevention goals at multiple joints. Third, we increased the computational efficiency of the ODSG process to produce results in a clinically relevant time frame. These enhancements can have major implications since the ODSG process can now find its way into clinical application. Our work also tested the enhanced ODSG process on both aerial and grounded movements and tested its ability to address both upper and lower body based biomechanical parameters.

1.3. Research innovation

Before using simulation platforms to find optimal simulations, we need to ensure that the simulation platform represents the experimental data accurately in the computer environment. In dynamic simulations, residuals represent the difference between the external and inertial forces. These residuals essentially

represent collective errors in the simulation generation process. These errors could be caused at different stages during and before of the simulation generation process like data collection, data mining, inertial parameters. Understandably, some error/residuals are expected, but there needs to be a bound on the allowable residuals. Recommendations have been made in the literature based on a rule-of-thumb strategy that set bounds on the residuals (Hicks et al., 2015). In this work, we used a concept from robotics, called the zero moment point (ZMP) computations (Reinbolt and Donnelly, 2017a; Vukobratović and Borovac, 2004), to assess the dynamic consistency of simulations. We used this mathematical theory to develop new guidelines to test simulation residuals and hence accept or reject that simulation. This innovative method of assessing simulations for dynamic consistency speaks directly to what the residuals represent and addresses limitations of the existing residual threshold recommendations.

The current ODSG process also suffers from numerous limitations. It has only been used to reduce one dimensional loads, lacks a ground contact model which limited its ability to ensure dynamic consistency between external and inertial forces, and takes multiple days to find the optimal movement patterns (Donnelly et al., 2012c). This work features several innovative solutions to address these limitations.

First, since the ODSG process essentially tests different movement patterns to find the optimal one, the external forces applied to the system should change based on the tested movement pattern. Our work primarily dealt with external

forces applied through the ground. To find these dynamically consistent external forces, complex and computationally expensive foot-ground contact models are required (Jackson et al., 2016). We solved the limitation of the absence of foot contact model in computational musculoskeletal by using ZMP computations as an alternate computationally efficient foot contact model to generate external forces that are dynamically consistent with the inertial forces of the simulation. This innovative solution allows us to generate dynamically consistent external forces without having to use a real foot contact model. This concept is further discussed in chapter 3.

Second, the ODSG process has only been used to reduce the risk of injury by reducing loads on a single joint (Donnelly et al., 2012c). These methods cannot handle performance aspects. We solved this limitation by using a novel technique of tracking hypothetical target trajectories of the performance segments that feature high performance parameters. This tracking task forces the trajectories of the performance segments of the simulations to be closer to the hypothetical high-performance trajectory and can in turn force changes in kinematics of segments of all the either body. At the same time, since the simulations are subject to anatomical and dynamic constraints, the generated simulations are still feasible.

Third, performance and injury prevention goals are often contradictory, and the ODSG process has never been used to balance between them. For example, in volleyball spiking, one wants to increase the height and the forward velocity of the hitting hand, but at the same time reduce loads at the shoulder to prevent injury.

These goals are contradictory. We solved this limitation by using goal-oriented optimization methods in the ODSG process. This innovative solution enables users to control the simulations such that specific user-defined goals can be met at the same time. These goals can encompass both performance goals and injury prevention goals at multiple joints. This goal-oriented optimization technique encourages the process to continue looking for the optimal movement pattern until all the goals are met. Not only does this enable the process to achieve a performance-injury prevention balance, but it also enables the end user to easily define or change these goals to find optimal movement patterns that meet specific biomechanical needs.

Fourth, the ODSG process currently takes multiple days to find optimal movement patterns. While this is acceptable for research, it limits the clinical relevance of the technique. To address this issue, we used a different, computationally more efficient way of generating simulations called trajectory optimization (Dembia et al., 2021) in ODSG process. This innovative solution allows us to find optimal movement patterns in a matter of minutes and also use complex foot contact models (Sherman et al., 2011). These advances in the ODSG process have taken it to the level where a doctor or coach can collect movement data from a patient or athlete, find an optimal movement pattern, test the optimal movement pattern, adjust the goals as needed, and retest the movement in a single session lasting an hour or two, making this technique clinically relevant.

1.4. Research methods

The ODSG process involves multiple steps, as shown in Fig. 1.1. Before the ODSG process, data collection, model scaling and inverse kinematics are performed. In this work, we also use two different forms of the ODSG process. The following is a brief description of each step and both forms of the ODSG process performed in this work.

1.4.1. Data collection

Experimental data collection is the first step of the process. This can be performed in a laboratory environment (Dempsey et al., 2012) or in the field (Saini et al., 2019). Multiple data collection tools can be used based on the movement, feasibility, and accuracy requirements. Some examples of motion capture tools are the gold standard of putting reflective markers on the participant whose movements are then captured by special cameras (Dempsey et al., 2012). Other motion capture equipment like inertial measurement units that detect movement using accelerometers and gyroscopes (MacDonald et al., 2017), and video cameras (Bishop and Hay, 1979) have also been used. All the data used in this work were collected in a laboratory environment using marker-based motion capture.

1.4.2. Model scaling

In order to create a simulation of the participant's movement, various platforms such as OpenSim (Delp et al., 2007) and AnyBody (Damsgaard et al., 2006) can be used. In this work we used OpenSim. Models of the human body in

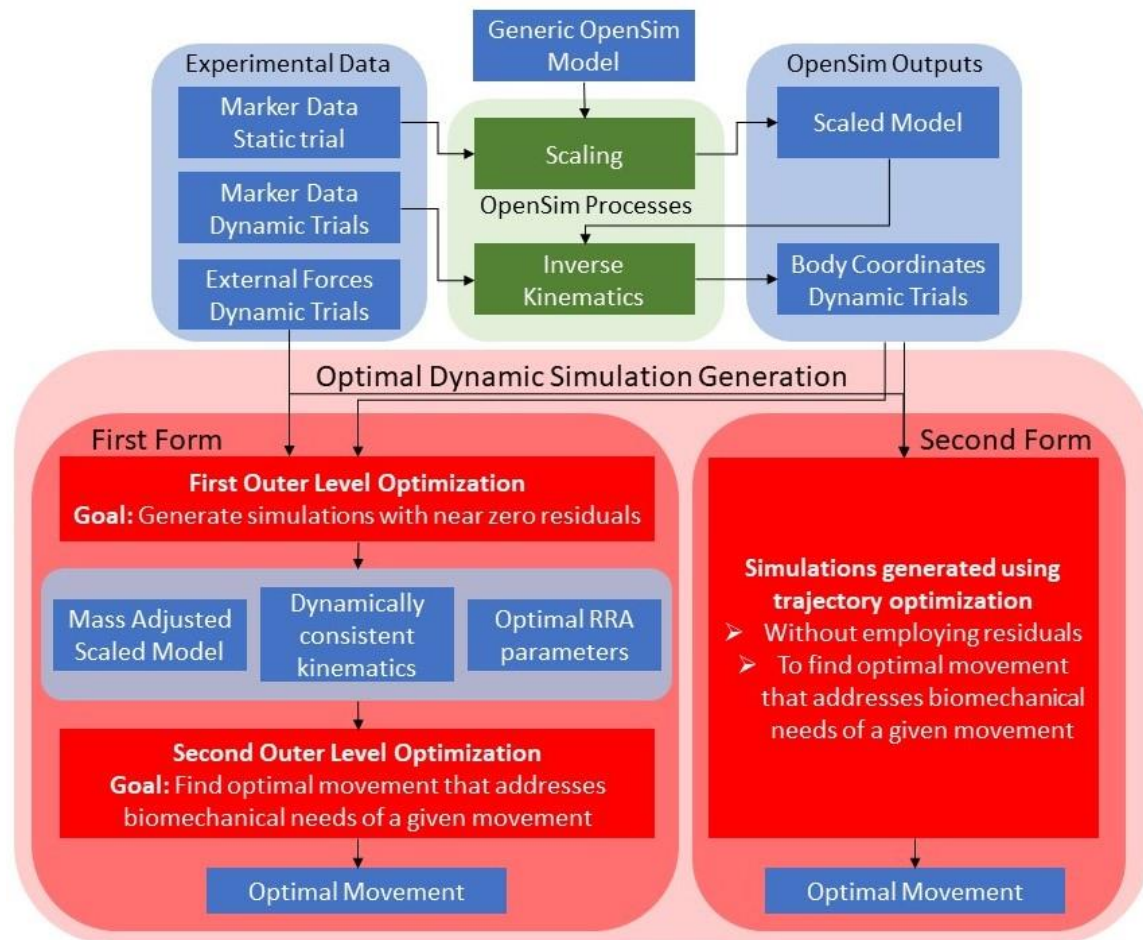


Figure 1.1. Flowchart of optimal dynamic simulation generation processes to find optimal movement patterns.

the OpenSim environment are freely available (www.simtk.org). These models encapsulate human anatomy and define inertial properties of each segment of the body, based on anthropometric data available in literature (de Leva, 1996; Winter, 2009). These models are scaled to the participant from whom the data is collected. This step uses marker data from a static posture of each participant. Additionally, this step appropriately assign the marker positions on the scaled model (Delp et al., 2007; Donnelly et al., 2021).

1.4.3. Inverse kinematics

After obtaining a scaled model, the next step is to perform inverse kinematics to get the body joint angles for the experimental data's movement trials. This step matches the position of each marker on the model to its position in the experimental movement trial. This is achieved through an optimization that adjusts the joint angles of the body such that the squared sum of error at each time frame between each marker's experimental versus simulation position is minimal. This gives us the joint angles at each time frame, referred to as the body coordinates (q). By adjusting the marker tracking weights, we can also choose which markers should be tracked more heavily compared to others (Delp et al., 2007).

1.4.4. Inverse dynamics

Inverse dynamics is an optional step that can be performed to estimate the overall torques at each joint. This step uses the body coordinates determined by inverse kinematics (q) and the distal external forces, such as the interaction forces between the ground and the foot that can be measured using a force plate, to find

the net torques about each body coordinate (τ) using classical equations of motion at each body segment (Delp et al., 2007).

$$M(q)\ddot{q} + C(q, \dot{q}) + G(q) = T \quad (1.1)$$

Where, $M(q)$ is the mass matrix, $C(q, \dot{q})$ represent the Coriolis and centrifugal forces, $G(q)$ are the gravitational forces and T are the net joint torques.

1.4.5. Residual reduction algorithm

Inverse dynamics applies the classical equations of motion sequentially from the distal to the proximal segments of the body. This causes errors to accumulate from distal to proximal ends. These errors, called residuals, are generally applied at the pelvis segment. The residual reduction algorithm implies a different approach to find net joint torques to minimize the residuals. Residual reduction algorithm (RRA) assumes that there are motors in each joint that drive the motion. The excitation/use of each of these motors, also referred to as actuators, correspond to the respective joint's net torque. RRA solves for the excitation of all these motors at the same time, rather than the sequential pattern that inverse dynamics uses. RRA still uses actuators for the residuals to reach dynamic consistency but minimizes their use. Additionally, RRA adjusts the body kinematics and model mass to increase dynamic consistency and reduce residuals. RRA minimizes the following cost function at each time frame (Delp et al., 2007; Thelen and Anderson, 2006):

$$\min_{x^R, x^T} \left[\sum_{i=1}^{n_q} w_{\ddot{q}_i} (\ddot{q}_i^{exp} - \ddot{q}_i^{sim})^2 + \sum_{j=1}^6 \left(\frac{R_j(x_j^R)}{R_j^{max}} \right)^2 + \sum_{k=1}^{n_T} \left(\frac{T_k(x_k^T)}{T_k^{max}} \right)^2 \right] \quad (1.2)$$

Where, x^R and x^T are the excitation levels (control magnitude) of the force and torque actuators. $\ddot{q}^{exp}$ and $\ddot{q}^{sim}$ are the experimental and simulation generated accelerations and $w_{\ddot{q}}$ are the tracking weight of the n_q degrees of freedom (number of joints (n_T) + number of residuals). R are the 6 residuals (three forces and three torques), T are the torques generated by the n_T torque generators, and R^{max} and T^{max} are maximum possible values for residuals and joint torques, respectively.

Note that even though RRA reduces the residuals, it still has some errors since it still uses residuals to achieve dynamic consistency. These errors or residuals are a combined sum of errors at various steps of the process such as accuracy of the data collection equipment, errors in scaling, how well the anthropometric data represents the participant, how well the RRA parameters like weights on each coordinate's tracking and the maximal torque producing capacity of the torque actuators represent the participant. We studied how much these residuals affect the dynamic consistency of a simulation in chapter 2.

1.4.6. Optimal dynamic simulation generation

The ODSG process performs two tasks: a) reduce residuals to ensure that the simulations are dynamically consistent, and b) generate simulations with the optimal movement pattern to addresses biomechanical needs of the given motion. In this work, we employed two forms of the ODSG process.

1.4.6.1. First form of optimal dynamic simulation generation

The first form of the ODSG process, used in chapters 3 and 4, generates simulations using the RRA. This RRA is controlled by another optimization called

the outer-level optimization (Reinbolt et al., 2011). The outer-level optimization is performed twice. The first implementation of the outer-level optimization adjusts the human-defined parameters of RRA to generate simulations with near zero residuals. This step essentially adjusts the simulation parameters to better represent each participant. Once each participant's simulation parameters have been optimized, ensuring virtually error free simulations, the second implementation of the outer-level optimization finds the optimal movement patterns. The outer-level optimization could be either a local or global optimization. Chapter 3 uses local optimization for the outer-level optimization, while chapter 4 uses local optimization in the first implementation of outer-level optimization (Donnelly et al., 2012c) and global optimization in the second (Goffe et al., 1994). Global optimization finds the best possible values of the parameters being tested, also called design variables, but computationally costlier and can ideally handle only limited number of design variables. Local optimization, on the other hand, finds values of design variables that are usually close to an initial guess specified by the user. While these “optimal” values of the design variables might not be the best possible values, this technique is computationally more efficient and ideal for optimizing a large number of design variables simultaneously. We used additional checks to ensure that the results from local optimization routines were good.

1.4.6.2. Second form of optimal dynamic simulation generation

The second form of the ODSG process, used in chapters 5 and 6, generates the simulations that are similar to the ones generated by RRA, but using a different

optimization algorithm called trajectory optimization. RRA performs optimization at each time frame in chronological order to find the excitation of each actuator at each time frame independently. This implies that RRA is incapable of adjusting the joint torques for an event that is about to happen. This is different from how humans determine joint torques. For example, if one is about to land after a jump, he/she starts contracting leg muscles before actually hitting the ground to help absorb the shock. This is another reason that residuals are present in RRA. The alternate simulation-generating algorithm, trajectory optimization, finds the excitation of each actuator at all time frames collectively, rather than analyzing each time frame independently (Dembia et al., 2021). Since all the time points are considered at the same time, the algorithm obtains a preview into the future, similar to humans using their senses, and adjusts joint torques accordingly. Trajectory optimization has multiple advantages: a) it resembles human decision making more closely than RRA, b) it reduces the need for residuals and c) since this algorithm considers all time points simultaneously rather than each time point individually, it is much faster than RRA.

OpenSim Moco is a new software designed to implement trajectory optimization to generate dynamic simulations (Dembia et al., 2021). In chapters 5 and 6, we used OpenSim Moco to generate simulations, combined with our knowledge of generating optimal movement patterns used in chapters 3 and 4. Since simulations generated using trajectory optimization do not necessarily need residuals, it also removes the need for the first implementation of outer-level

optimization, the step which is meant to reduce residuals (Fig. 1.1). This makes finding optimal movement patterns a single step process.

1.5. Structure of this work

This work comprises four studies designed to both enhance the ODSG process in a progressive manner and solve real-life biomechanical needs of a variety of movements. These movements span both aerial and grounded movements and examine biomechanical needs of both upper and lower body segments. Fig. 1.2. describes the goals and innovation of each study.

1.5.1. Study I: Physics-based guidelines for accepting reasonable dynamic simulations of movement

Goal: Understand the effect of residuals on dynamic consistency of dynamic simulations, establish physics-based guidelines to assess dynamic consistency, and consequently accept or reject simulations.

Methods: Integrate the robotics concept of ZMP computations to mathematically measure the effect of residuals on the dynamic consistency of simulations and set guidelines to accept or reject simulations by establishing limits based on physics-based acceptable ranges of dynamic consistency.

Significance: The guidelines established in this study are applicable to any movement and give the broader simulation community a tool to assess the dynamic consistency of their simulations.

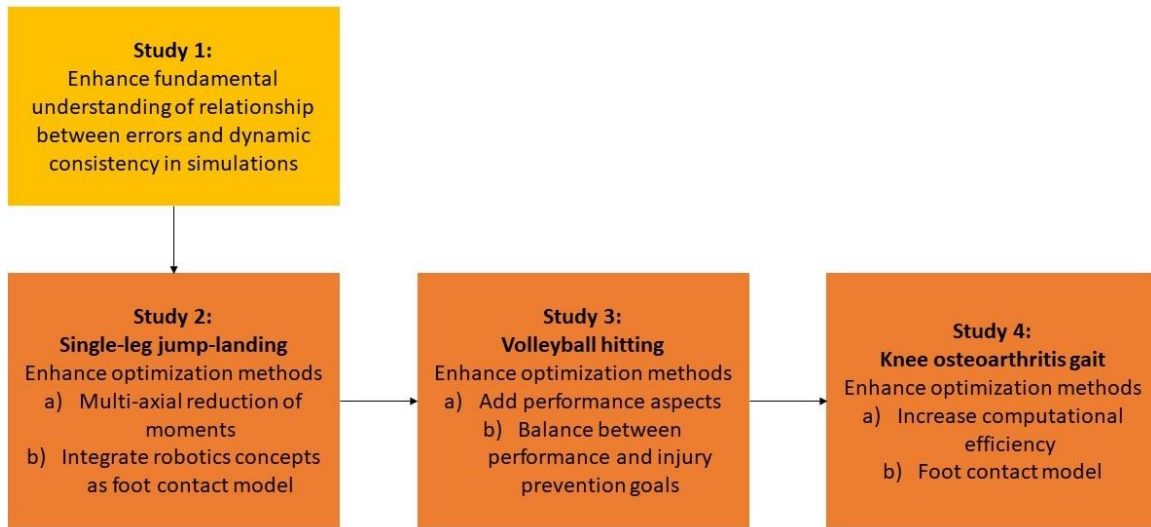


Figure 1.2. Flowchart of the studies in this work.

1.5.2. Study II: Optimal whole-body kinematics during single-leg jump-landing to reduce peak ab/ad-duction and internal rotation knee moments: Implications for anterior cruciate ligament injury risk

Goal: Find optimal whole-body, participant-specific movement patterns that reduce the risk of ACL injury during single-leg jump-landing.

Methods: We used the first form of the ODSG process and enhanced it by integrating ZMP computations to increase dynamic consistency of simulations.

Significance: In each variation of the movement, the interaction between the foot and the ground changes, which in turn changes the forces experienced through the ground. Previously, the absence of a foot contact model in the ODSG process limited its ability to find ground reaction forces that are dynamically consistent with each variation of the movement tested. Integration of the ZMP computation solved this problem and enhanced the robustness of the ODSG process. Additionally, this study's findings can lead to the establishment of new training protocols for athletes that help reduce the risk of ACL injury during landing.

1.5.3. Study III: Use of goal-oriented optimization of dynamic simulations to find a balance between performance and injury prevention balance during volleyball spiking

Goal: Find optimal whole-body, participant-specific movement patterns for volleyball spiking that enhances performance and reduce the risk of shoulder injury simultaneously.

Methods: We used the first form of the ODSG process and enhanced it by adding methods to control performance aspects. Additionally, we introduced goal-oriented optimization methods that can be programmed to suit specific performance and injury prevention needs. Moreover, we expanded the ODSG process to be able to incorporate performance and injury prevention needs at multiple joints of the body.

Significance: This study broadened the ability of the ODSG process to be able to address multiple biomechanical parameters at the same time, which is essential for a robust system. Moreover, the ability to easily incorporate participant-specific needs using our goal-oriented optimization approach makes it customizable and hence more robust for a variety of applications.

Another significance of this study is that it proved that performance and injury prevention are not mutually exclusive. This directly contradicts the common belief that performance and injury prevention are mutually exclusive. This can potentially change the way training protocols are designed sports and musculoskeletal rehabilitation.

From the perspective of application, is significant as it found movement patterns that volleyball athletes can use to enhance performance without increasing risk of injury. Additionally, the discovered underlying mechanism driving these changes can be used to establish new training protocols.

1.5.4. Study IV: Optimal gait patterns that reduce peak knee adduction moment without increasing peak knee flexion/extension moment:

Implications for progression of knee osteoarthritis

Goal: Find optimal whole-body, participant-specific gait patterns that reduce the progression of knee osteoarthritis.

Methods: We used the second form of the ODSG process that employs trajectory optimization to generate simulations. We integrated the aspects of the first form to make the second form capable of finding optimal movement patterns. Additionally, we integrated a foot contact model to increase the dynamic consistency of the tested movement patterns, since foot contact models are better at modeling foot-ground interactions than ZMP computations.

Significance: The second form of the ODSG process has been used to generate simulations, but never to find optimal movement patterns. Our integration of the concepts from the first form enables the second form to achieve this. Since the second form uses a faster one-step process to find optimal movement patterns, it was able to reduce the computational time of the ODSG process from multiple days in the first form to mere minutes. This overcomes the final obstacle using the ODSG process practically and thus gains clinical relevance. Moreover, this study can lead to rehabilitation protocols that can help restrict the progression of knee osteoarthritis.

CHAPTER TWO

STUDY I: PHYSICS-BASED GUIDELINES FOR ACCEPTING REASONABLE DYNAMIC SIMULATIONS OF MOVEMENT

2.1. Abstract

In dynamic simulations, residuals are nonphysical generalized forces that a) dynamically balance externally applied and inertial forces and moments and b) account for data processing and modeling errors. Hicks, et al. (2015) proposed the original residual threshold recommendations for an acceptable simulation, but these thresholds do not account for the dynamic, physics-based movement characteristics.

In this study, we present three new, physics-based guidelines for accepting reasonable dynamic simulations of movement using zero moment point (ZMP) computations and thresholds for forces, center of pressure, and free moment. We evaluated our new guidelines alongside the original 2015 recommendations using two purposefully different movements: single-leg jump-landing (SLJL) and walking gait. We present a MATLAB function for others to test if their simulations meet the new guidelines.

For our chosen movement data, we found only 4.3% (SLJL) and 8.2% (gait), on average, of the original 2015 residuals volume met all the new physics-based guidelines. Additionally, some of the new recommended residuals volume falls outside of the original 2015 recommendations. Particularly, the free-moment guideline was the most restrictive for reasonable simulations, especially for high-velocity movements at times with lower vertical ground reaction forces. Moreover, accepting reasonable simulations using different thresholds leads to different joint torques as high as 24 Nm (SLJL) and 8.2 Nm (gait), on average, which may lead

to different conclusions and clinical interpretations. We advocate the use of these new guidelines as they are overall more restrictive than the original 2015 ones and accept only reasonable simulations considering the dynamic, physics-based characteristics of the movement.

2.2. Introduction

In musculoskeletal modeling simulations, residual forces and moments (residuals) are referred to as “hand of god” nonphysical generalized forces and they are necessary to dynamically balance the difference between the externally applied and inertial forces and moments (Hicks et al., 2015; Reinbolt et al., 2011). Practically, residuals represent how well the human or animal movement is recorded, processed, and modelled in the *in silico* environment. Since it is extremely difficult to perfectly model a movement *in silico*, some residuals (or errors) are expected. It is, however, necessary to understand how much of this error is physically allowable in the simulations (Delp et al., 2007; Hicks et al., 2015; Reinbolt et al., 2011) because it affects the validity of the conclusions and subsequent clinical interpretations derived from the simulation studies.

Initial recommendations have been made on thresholds for residuals during walking and running simulations (Hicks et al., 2015) and on the OpenSim online documentation (www.simtk.org). Hicks, et al. (2015) recommended that residual forces should be below 5% (peak and RMS) of the experimental net external force magnitude and residual moments should be below 1% of the center of mass (COM) height times the experimental net external force magnitude. These first-

generation recommendations served as a valuable reference for the simulation community, but they have certain limitations. First, these recommendations are based on a rule of thumb rather than on dynamic, physics-based characteristics of the movement itself. Second, these single-threshold values for the force and moment limits are used during all phases of the movement. Third, these limits are based on the measured net external force magnitude to establish thresholds for all six residual components (3 forces and 3 moments) even though these components are independent from each other. To address these limitations, new physics-based guidelines are needed to set independent residual thresholds that can be applied to different phases of movement.

One powerful mathematical approach to establish relationships between residuals and ground reaction forces (GRF) is zero moment point (ZMP) computations (Reinbolt and Donnelly, 2017a; Xiang et al., 2010; Xiang et al., 2009). Residuals and experimental GRF are both external forces and moments applied to the dynamic system at two different points. Consequently, it is imprudent to establish the residual moment threshold based on the height-scaled experimental GRF force magnitude alone because residuals can vary at different applied points. ZMP computations use a force and moment balance to transform a set of forces and moments applied at any point on the system to a dynamically equivalent set applied at a globally defined point on the ground known as the ZMP. Given a set of forces and moments ($\bar{F}_p$ and $\bar{M}_p$) applied at the pelvis ($\bar{r}_p$), the equivalent forces and moments ($\bar{F}_{ZMP}$ and $\bar{M}_{ZMP}$) applied at the ZMP ($\bar{r}_{ZMP}$) are:

$$\bar{F}_{ZMP} = \bar{F}_p \quad (2.1)$$

$$\bar{M}_{ZMP} + \bar{r}_{ZMP} \times \bar{F}_{ZMP} = \bar{M}_p + \bar{r}_p \times \bar{F}_p \quad (2.2)$$

Since the $\bar{F}_{ZMP}$ and $\bar{M}_{ZMP}$ are applied at the ground, $\bar{M}_{ZMP}$ consists of only the free moment, or the vertical component, such that $\bar{M}_{ZMP} = (0, MY_{ZMP}, 0)$, and $\bar{r}_{ZMP}$ does not have a vertical component, such that $\bar{r}_{ZMP} = (X_{ZMP}, 0, Z_{ZMP})$. Hence,

$$X_{ZMP} = f(MZ_p, FX_p, FY_p) = X_p + \frac{(MZ_p - Y_p FX_p)}{FY_p} \quad (2.3)$$

$$Z_{ZMP} = g(MX_p, FZ_p, FY_p) = Z_p - \frac{(MX_p + Y_p FZ_p)}{FY_p} \quad (2.4)$$

From Eq. 2.1-2.4,

$$MY_{ZMP} = g(FX_p, FY_p, FZ_p, MX_p, MY_p, MZ_p) = MY_p + \frac{FX_p MX_p}{FY_p} + \frac{FZ_p MZ_p}{FY_p} \quad (2.5)$$

In this study, we used ZMP computations as the mathematical framework to compare the residuals to the experimental GRF and the nature of well understood physical quantities like center of pressure (COP) and GRF to establish thresholds to accept or reject residuals. We combined the two sets of external forces and moments (residuals and experimental GRF) to find a single set of net external forces and moments (ZMP forces and moments), applied at a point on the ground (ZMP). If the residuals are exactly zero, the ZMP forces and moments are identical to the experimental GRF, and the ZMP coincides with the COP. However, when residuals are nonzero, they cause the ZMP forces and moments to deviate from the experimental GRF and the ZMP to deviate from the COP. For a given movement and foot-ground contact surfaces, ZMP forces and moments that

deviate too far from the experimental GRF forces and moments are physically unreasonable. Additionally, a ZMP too far from the COP could even be outside of the base of support, which is also physically unreasonable. We use these principles to recommend a new set of residual thresholds to accept reasonable simulations considering the dynamic, physics-based characteristics of the movement.

There are three main parts to this study. First, we used ZMP computations to establish the mathematical relationships between residuals and experimental GRF to make three new guidelines on residual thresholds to compare with the original 2015 recommendations. Second, we present a MATLAB function that the community can use to test our new guidelines. Third, to demonstrate the effect of implementing different threshold recommendations, we compared the residuals and kinetics of two different simulations of the same movement, one satisfying our new residual thresholds and another satisfying the original 2015 thresholds. A preliminary version of this work, partially describing one of the three new guidelines, has been reported (Gupta et al., 2019a).

2.3. Methods

2.3.1. Mathematical approach, new threshold guidelines, and comparison to the original 2015 recommendations

2.3.1.1. Mathematical relationships between residuals and experimental ground reaction forces

Let $\bar{F}_p(FX_p, FY_p, FZ_p)$ and $\bar{M}_p(MX_p, MY_p, MZ_p)$ represent the set of forces and moments equivalent to only the experimental GRF forces ($\bar{F}_{GRF}$) and moments ($\bar{M}_{GRF}$) applied at the pelvis. When transformed using ZMP computations, the $\bar{r}_{ZMP}$, $\bar{F}_{ZMP}$, and $\bar{M}_{ZMP}$ would be identical to the experimental COP, $\bar{F}_{GRF}$, and $\bar{M}_{GRF}$, respectively. Residuals change the external forces and moments at pelvis. Hence, the residual forces $\Delta\bar{F}_p(\Delta FX_p, \Delta FY_p, \Delta FZ_p)$ and residual moments $\Delta\bar{M}_p(\Delta MX_p, \Delta MY_p, \Delta MZ_p)$ cause the $\bar{r}_{ZMP}$, $\bar{F}_{ZMP}$ and $\bar{M}_{ZMP}$ to deviate from the experimental COP, $\bar{F}_{GRF}$, and $\bar{M}_{GRF}$. These deviations ($\Delta\bar{r}_{ZMP}(\Delta X_{ZMP}, 0, \Delta Z_{ZMP}), \Delta\bar{F}_{ZMP}$, and $\Delta\bar{M}_{ZMP}(0, \Delta MY_{ZMP}, 0)$) can be mathematically expressed by using partial differentiation on Eq. 2.1, 2.3-2.5.

$$\Delta\bar{F}_{ZMP} = \Delta\bar{F}_p \quad (2.6)$$

$$\Delta X_{ZMP} = \frac{1}{FY_p} \left(\Delta MZ_p - Y_p \Delta FX_p - \frac{(MZ_p - Y_p FX_p) \Delta FY_p}{FY_p} \right) \quad (2.7)$$

$$\Delta Z_{ZMP} = \frac{1}{FY_p} \left(-\Delta MX_p - Y_p \Delta FZ_p + \frac{(MX_p + Y_p FZ_p) \Delta FY_p}{FY_p} \right) \quad (2.8)$$

$$\Delta MY_{ZMP} = \Delta MY_p + \frac{1}{FY_p} \left(\begin{aligned} &FX_p \Delta MX_p + MX_p \Delta FX_p \\ &+ FZ_p \Delta MZ_p + MZ_p \Delta FZ_p \\ &- \frac{(FX_p MX_p + FZ_p MZ_p)}{FY_p} \Delta FY_p \end{aligned} \right) \quad (2.9)$$

These equations allow us to mathematically compute the effect of residuals on well understood physical quantities of COP, GRFs, and free moment.

2.3.1.2. New threshold guidelines to accept or reject reasonable simulations

Based on the physical nature of the COP and GRF, we set new residual threshold guidelines. Due to the physics of a given movement and foot-ground contact surface friction, it is physically unreasonable to have large quantities of

$\Delta \bar{F}_{ZMP}$ and $\Delta \bar{M}_{ZMP}$. Additionally, a large $\Delta \bar{r}_{ZMP}$ represents net external forces and moments applied at a point that might not even be within the base of support, which is also physically unreasonable. By establishing reasonable bounds on the allowable change in the COP, total external forces, and the total free moment, we can accept or reject a simulation based on their residuals. We recommend thresholds to be tested at each time frame of the simulation and deemed unacceptable for that time frame if any of the following threshold guidelines are violated:

1) Force guideline

The difference between the total external forces and the experimental $\bar{F}_{GRF}$, that is $\Delta \bar{F}_{ZMP}$ (which is equal to $\Delta \bar{F}_p$ (Eq. 2.6), is less than $a(a_x, a_y, a_z)\%$ of the peak magnitude of experimental $\bar{F}_{GRF}(FX_{GRF}, FY_{GRF}, FZ_{GRF})$ in each direction independently.

$$\Delta FX_p < \frac{a_x}{100} * \max(|FX_{GRF}|), \Delta FY_p < \frac{a_y}{100} * \max(|FY_{GRF}|), \Delta FZ_p < \frac{a_z}{100} * \max(|FZ_{GRF}|) \quad (2.10)$$

2) ZMP guideline

Distance between the ZMP the experimental COP is less than d .

$$\sqrt{\Delta X_{ZMP}^2 + \Delta Y_{ZMP}^2} < d \quad (2.11)$$

3) Free moment guideline

The difference between ZMP free moment and experimental free moment is less than $b\%$ of the peak magnitude of experimental GRF free moment.

$$\Delta MY_{ZMP} < \frac{b}{100} * \max(|MY_{GRF}|) \quad (2.12)$$

For this study, we used $a_x = 10\%$, $a_y = 5\%$, $a_z = 10\%$, $d = 5\text{ cm}$, and $b = 10\%$. Since the vertical GRF is not influenced by the foot-ground friction as is the horizontal GRF forces and free moment, the value of a_y was chosen to be lower than those of a_x, a_z and b . The distance, d , was selected to allow the ZMP to remain under the base of support.

2.3.1.3. New and original 2015 threshold recommendations

In this study, we used data from two different movements, single-leg jump-landing (SLJL) data collected at The University of Western Australia (Dempsey et al., 2012) and split belt treadmill gait data freely available with the OpenSim software (simtk.org). For SLJL, we used data from the weight acceptance phase, that is start of foot contact to the ground till the first local minimum in the vertical experimental GRF force (Brown et al., 2014b). The weight acceptance phase was chosen because it is the time when the athlete is most vulnerable to ACL injury (Donnelly et al., 2012c). For gait, we used data of one complete gait cycle. For the double stance phase, the $\Delta\bar{F}_{ZMP}$, $\Delta\bar{M}_{ZMP}$ and $\Delta\bar{r}_{ZMP}$ represent the deviation in ZMP forces, ZMP free moment and ZMP from the resultant experimental GRF forces, free moment and COP (which would lie somewhere between the two feet). These two motions help us understand the effect of residuals on both high- and low-velocity movements.

For each movement, we established the 6-D space of acceptable residuals based on the original 2015 recommendations (2015 residuals volume). We sampled residual combinations in a grid pattern from a space 50% larger than this

2015 residuals volume. At each time frame of the movement, we tested each residual combination to check if it satisfies one of four combination of recommendations: 1) 2015 only, 2) new ones only, 3) both 2015 and new together, or 4) neither 2015 or new ones.

Residual force and moment thresholds of the original 2015 recommendations independently establish limits on the residual force vector magnitude (a spherical volume of allowable residual forces) and the residual moment vector magnitude (a spherical volume of allowable moments). However, both residual forces and moments affect $\Delta \bar{r}_{ZMP}$ and $\Delta \bar{M}_{ZMP}$ (Eq. 2.7-2.9). Therefore, in the new guidelines, residual forces and moments cannot be tested independent of each other. For this reason, we sampled residual combinations from a 6-D space of residuals.

2.3.2. MATLAB function for the new threshold guidelines

We developed a MATLAB function, `checkGuidelines.m` (Supplementary data 2.4), that the community can use to test if their simulation residuals violate the new guidelines. The function inputs are the simulation residuals and kinematics, experimental GRF, time range for testing residuals, and threshold values of a , d , and b . The function implements ZMP computations and tests when the simulation residuals violate any of the new guidelines and generates a visual representation of these results. For demonstration purposes, the SLJL and gait data described earlier were used to generate simulations of each movement and the residuals from the Residual Reduction Algorithm (RRA) and the gait2392

model scaled to each participant using the OpenSim software (simtk.org) were tested. We added arms (Hamner et al., 2010) to generate a full-body model. For SLJL simulation in this analysis, we locked the subtalar and metatarsophalangeal (MTP) joints for computational efficiency, and used a 3 degree of freedom knee (Donnelly et al., 2012c) since SLJL is prone to ACL injury and knee adduction and internal rotation moment are predictors of ACL injury.

2.3.3. Different threshold recommendations may change simulation results

Different threshold recommendations will likely change the accepted simulation kinetics. To study the effect of following the new guidelines as opposed to the original 2015 recommendations, we ran two outer-level optimization routines on SLJL and gait data (Reinbolt et al., 2011). The outer-level optimization uses an optimization routine to control parameters of a simulation generation process, in this case RRA. The design variables for the optimization routines were the model's capacity to produce residuals and this capacity was slowly reduced until the RRA results met the desired recommendations. For the gait simulations, we only ran the optimization routines for half gait cycle and locked the subtalar and MTP joints for computational efficiency. For both SLJL and gait optimizations, the first optimization was run until all the original 2015 recommendations were met and the second optimization was run until all the new guidelines were met. The initial guess was the same for both the optimizations. We evaluated the differences in the external forces and moments as well as the external impulse between the two accepted simulations. These differences represent the differences in simulation

residuals because these are the only external forces and moments that differ between the two accepted simulations. We also evaluated the subsequent change in model kinetics between the two accepted simulations.

2.4. Results

2.4.1. New threshold guidelines compared to the original 2015 recommendations

The new threshold guidelines for simulations of different movements establish a direction-independent acceptable threshold volume unlike the original 2015 recommendations that base thresholds on a single value for the magnitude of the experimental $\bar{F}_{GRF}$ (Fig. 2.1.a-b). The new guidelines compare the magnitude of each residual force component to $\alpha\%$ of peak magnitude of the corresponding experimental GRF force in that respective component direction, which results in a cuboid shape of allowable force volume. However, the original 2015 recommendations put a threshold on the magnitude of the residual force vector, which results in a different, larger spherical shape of allowable force volume. On average, 43.4% and 15.8% of the 2015 residuals volume overlapped with the new cuboid volume for SLJL and gait, respectively (Fig. 2.1.c-d).

The three new threshold guidelines extend the static-only force threshold of the original 2015 recommendations with two dynamic guidelines that vary with time (Fig. 2.1.c-d). The force guideline, albeit direction independent, is static and depends on the peak magnitude of experimental $\bar{F}_{GRF}$ over the whole movement (Eq. 2.10). On the other hand, ZMP and free moment guidelines are dynamic and

depend on the trajectories of components of the experimental GRF (Eq. 2.7-2.9, 2.11-2.12). On average, 71.3% and 89.8% of the 2015 residuals volume met the ZMP guideline and 10.0% and 48.1% met the free moment guideline for SLJL and gait, respectively (Fig. 2.1.c-d). Overall, on average, 4.3% and 8.2% of the 2015 residuals volume met all of the three new guidelines for SLJL and gait, respectively (Fig. 2.1.c-d). Supplementary data 2.1.A-B display the dynamic nature of the new guidelines and compare them to the original 2015 recommendations. The new threshold guidelines reduce the number of acceptable simulations in the residuals volume compared with the 2015 residuals volume because a number of residuals combinations place the ZMP outside the base of support or generate a free moment larger than possible without the foot sliding on the ground (Fig. 2.1.e-f). Moreover, there were even fewer acceptable simulations in the residuals volume that met both the new and original 2015 recommendations.

2.4.2. MATLAB function outputs

Supplementary data 2.2.A-B present the MATLAB results of ZMP computations and when each of the three guidelines are violated during the movement for SLJL and gait. For the SLJL simulation, at least one of the new guidelines was always violated over the movement timeline. For the gait simulation, the force and ZMP guidelines were almost always met and the free moment guideline was almost always violated over the gait cycle.

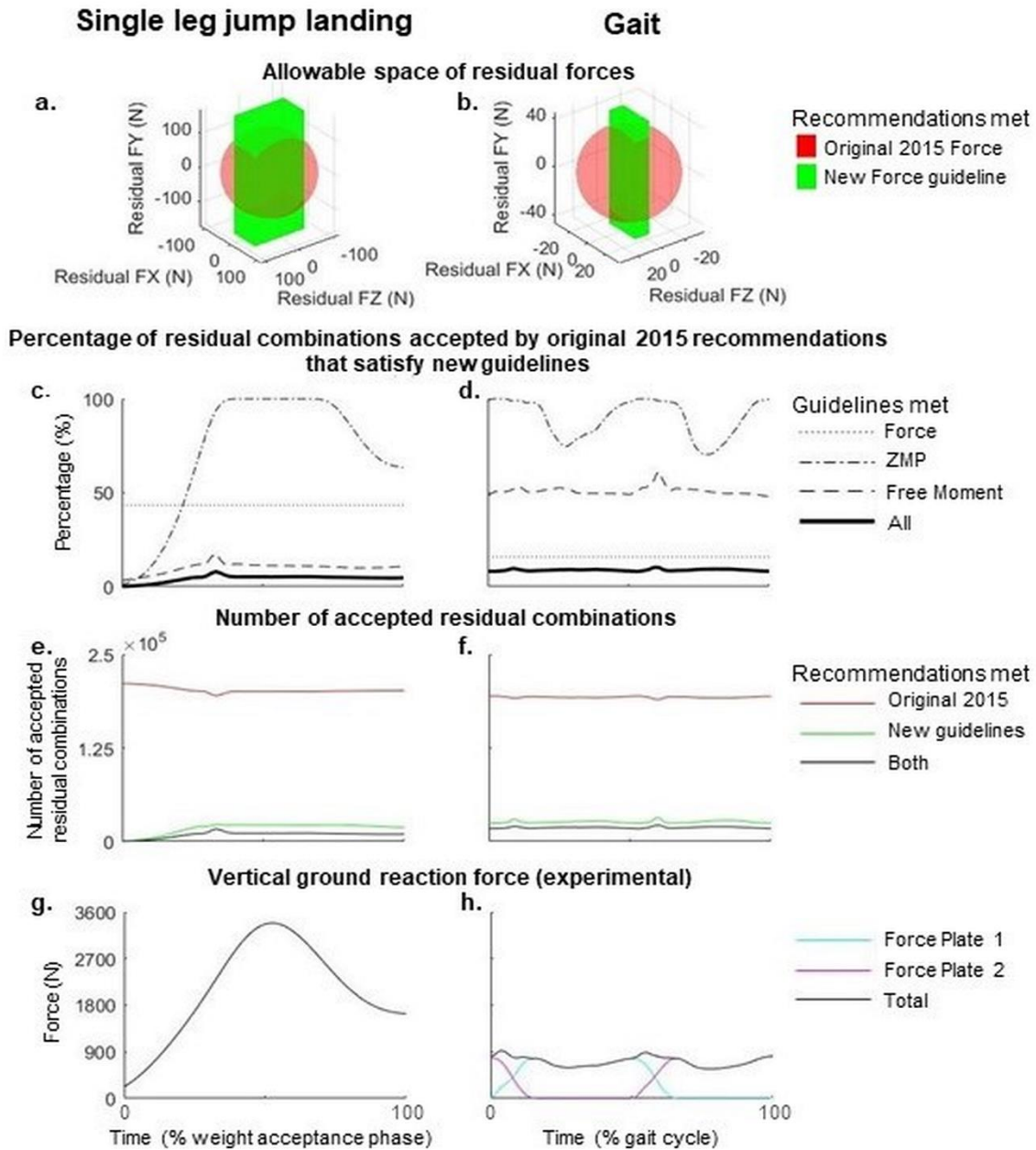


Figure 2.1. Behavior of new guidelines compared to the original 2015 recommendations for single-leg jump-landing and gait. **2.1.a-b.** It is observable that a residual combination might satisfy either one, neither or both original 2015 and new force recommendations. SLJL has a larger volume than gait since SLJL has larger experimental ground reaction forces (2.1.g-h.). From our force guideline, the allowable residuals in M/L direction (Z) are larger than those in A/P direction (X) for SLJL while it is opposite for gait because SLJL has a larger peak magnitude of M/L GRF force compared to

peak magnitude of A/P GRF force, while the opposite is true for gait. On the other hand, the original 2015 recommendations treat all the 3 directions equally. **2.1.c-d.** The percentage of 2015 residuals volume accepted that satisfies our ZMP and free moment guidelines follow a pattern similar to the vertical experimental GRF force (2.1.g-h.). It is also observable that the ZMP guideline curve follows the pattern better than the free moment curve. **2.1.e-f.** Since the original 2015 recommendations are static over the movement, the number of combinations accepted by the original 2015 recommendations remain constant over the movement, hence the red and black lines are complimentary over the movement.

2.4.3. Effect of different threshold recommendations on simulation results

The new guidelines greatly restricted the threshold on the vertical moment residual, ΔMY_p , mainly due to the free moment guideline (as seen in Eq. 2.9). For both SLJL and gait, the simulations following the new guidelines had a considerably lower MY_p residual compared to the those following the original 2015 recommendations. We found that other residuals may or may not differ between the two different movement simulations (Fig. 2.2.a).

The changes in the external forces and moments (residuals) caused changes in simulation kinetics. Changes in joint torques as high as 24 Nm and 8.2 Nm were observed between the two simulations of SLJL and gait, respectively (Fig. 2.2.b). The kinematics of the two acceptable gait simulations differed from each other (Supplementary data 2.3.B). The two SLJL simulations, however, followed almost identical kinematics (Supplementary data 2.3.A). Even though the difference in the magnitudes of residuals between the two SLJL simulations was greater than that between the two gait simulations, kinematic differences were only observed between the two gait simulations because the SLJL simulations were much shorter (60 ms) compared to gait simulations (633 ms). The magnitude of difference in external impulse (impulse generated by the residuals) between the two gait simulations and between the two SLJL simulations was comparable (Fig. 2.2.a), but at the end of the simulations, the longer time period of the gait simulations resulted in more differences in kinematics. Supplementary data 2.3.A-

B illustrates the differences in the kinetics and kinematics between the two SLJL and the two gait simulations in detail.

2.5. Discussion

In this study, we demonstrated new physics-based guidelines for accepting dynamic simulations using mathematical principles to relate the residuals to the experimental GRF. We made three guidelines based on physical characteristics of a given motion and foot-ground contact to set the residual thresholds. Our new guidelines are dynamic and capable of adapting for different phases of a movement. We also developed a MATLAB function to aid implementation of these new guidelines and showed that following different sets of recommendations can produce different simulation kinetics.

2.5.1. Interpretation of differences between the new and original 2015 recommendations

For different dynamic movements, it is important to base residual thresholds on different force-component values rather than a single value. Only 43.4% (SLJL) and 15.8% (gait) of the 2015 residuals volume met the new force guideline (Fig. 1.c-d) because the original 2015 thresholds are based on a single force value (magnitude of experimental $\bar{F}_{GRF}$ vector). For most human movements, the vertical force contributes far more to the magnitude of experimental $\bar{F}_{GRF}$ compared to the horizontal components. For low-velocity movements like gait, peak magnitudes of horizontal components are less than 20% (roughly 15% A/P and 6% M/L) of the peak vertical component. By allowing all residual forces up to 5% of experimental

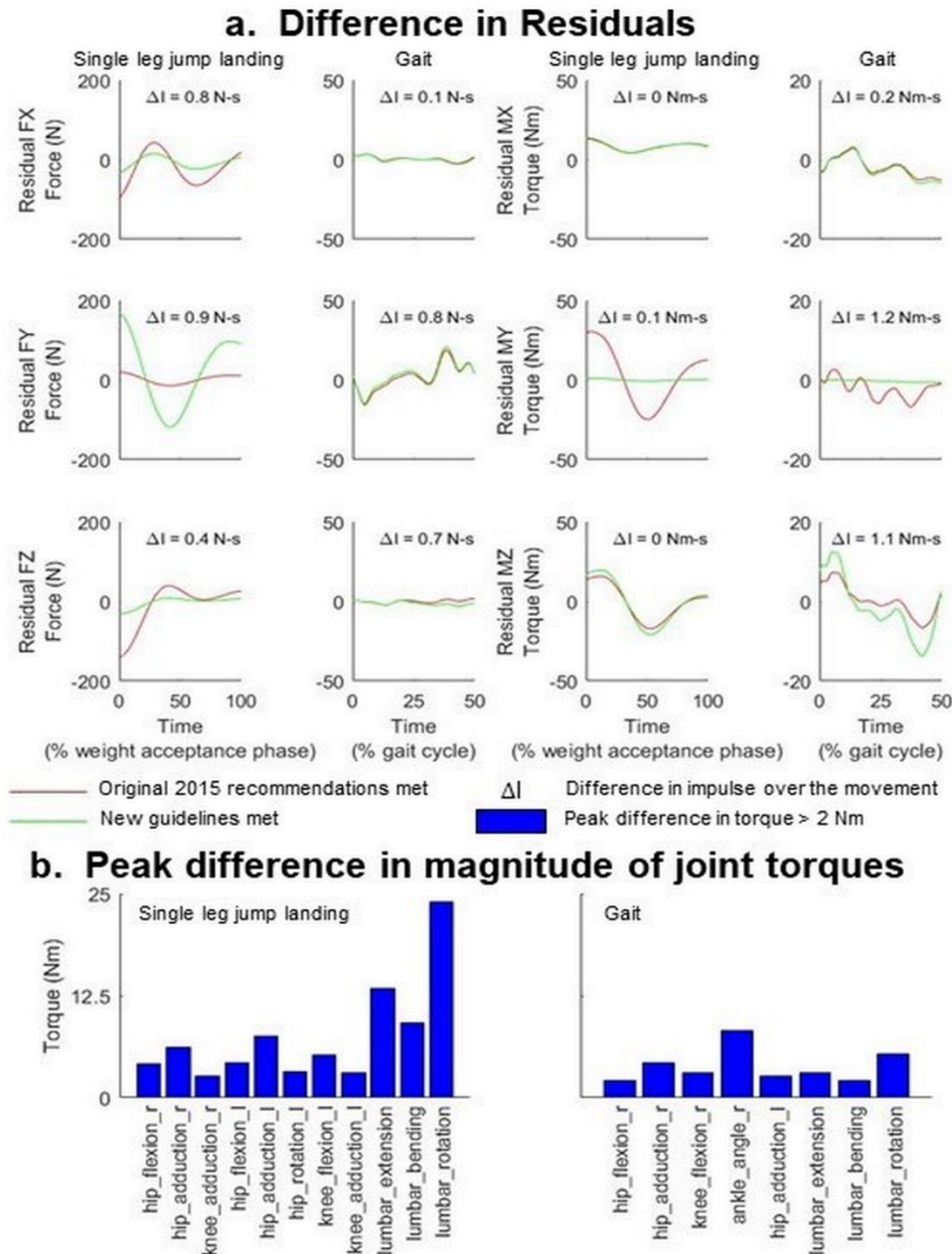


Figure 2.2: Difference between simulations following the original 2015 recommendations and the new guidelines for the same movement. **2.a.** The new guidelines are more restrictive on the residual MY since it directly influences the most restrictive free moment guideline (Eq. 2.9). **2.b.** Coordinates with peak differences in magnitude of joint torque greater than 2 Nm between the two simulations of SLJL and those of gait are depicted. Multiple joint torques differ between the two simulations of the same movement that follow different residual threshold recommendations.

$\bar{F}_{GRF}$ magnitude irrespective of the force direction, the original 2015 recommendations allow for horizontal residuals that are approaching peak magnitudes of the corresponding experimental $\bar{F}_{GRF}$, which is physically not achievable. The new and original 2015 recommendations agreed better for SLJL than gait because the SLJL peak horizontal GRF force components (roughly 12% A/P and 21% M/L) were a larger fraction of the vertical component compared to gait. This finding highlights the importance of the new force guideline for accepting reasonable simulations of low-velocity movements such as gait.

The vertical component of the experimental $\bar{F}_{GRF}$ vector directly influences the dynamic nature of the new guidelines. As the vertical GRF force increases, the new guideline thresholds increase as well and the likelihood of the simulation to be accepted increases (Fig. 2.1.c-h). This increase is a result of $\Delta\bar{r}_{ZMP}$ and most terms in ΔMY_{ZMP} being inversely proportional to the vertical experimental $\bar{F}_{GRF}$, FY_p (Eq. 2.7-2.9). All terms of $\Delta\bar{r}_{ZMP}$ are inversely proportional to FY_p (Eq. 2.7-2.8) while not all terms of ΔMY_{ZMP} are inversely proportional to FY_p (Eq. 2.9). For this reason, the shape of the curve representing percentage of the 2015 residuals volume that satisfies the ZMP guideline looks more similar to the shape of the vertical experimental $\bar{F}_{GRF}$ compared to the shape of the curve representing percentage of the 2015 residuals volume that satisfies the free moment guideline (Fig. 2.1.c-h).

The new free moment guideline is very important for high-velocity movements such as SLJL. The free moment is dependent on the movement

velocity and foot-ground friction parameters; however, experimentally, it does not necessarily increase when the vertical GRF force increases. In fact, the peak magnitude of experimental free moment for SLJL (20.5 Nm) was lower than that for gait (25.4 Nm) in the data described above. The original 2015 recommendations base the residual moment threshold on the participant-height-scaled magnitude of the experimental GRF force. This allows for a much larger volume for allowable residual moments for SLJL compared to that for gait. The residual ΔMY_p directly influences ΔMY_{ZMP} (Eq. 2.9) and a larger allowable volume of residual moments allows for larger values of ΔMY_{ZMP} for SLJL compared to gait (Supplementary data 1.A-B), even though the magnitude experimental free moment of both the movements is very similar. For this reason, the percentage of the 2015 residuals volume that met the new free moment guideline was higher for gait compared to SLJL (Fig. 2.1.c-d). Hence, the free moment it is very important for high-velocity movements.

The original 2015 recommendations allow for nonphysical free moments. Based on the original 2015 recommendations, the allowable range of ZMP free moment is higher at lower vertical experimental $\bar{F}_{GRF}$ (Supplementary data 2.1.A-B) since most terms of ΔMY_{ZMP} are inversely proportional to FY_p (Eq. 2.9). This scenario is physically unreasonable because the free moment is generated by friction, that directly depends on the vertical force. These results highlight the importance of the new free moment guideline.

Potentially, residuals can meet the new threshold guidelines and violate the original 2015 recommendations (Fig. 2.1.e-f) because certain residual terms in the ZMP computations can offset one another due to sign differences. For example, in Eq. 2.7, it is possible to have large ΔMZ_p (positive contribution) and large ΔFX_p (negative contribution) with an overall very small ΔX_{ZMP} . It is important to note that this case only means that the X_{ZMP} is close to X_{COP} .

2.5.2. MATLAB function

Our MATLAB function allows others to test the new guidelines and identify regions of the simulated movement where the new guidelines are being violated. The fact that the free moment guideline was almost always violated for both SLJL and gait (Supplementary data 2.2.A-B) suggest that it is more restrictive compared to the other two threshold guidelines. Additionally, the fact that the new force and ZMP guidelines were only violated for SLJL and not for gait suggest that these guidelines are more important for high velocity movements. Interestingly, this observation contradicts the result from the previous section that the force guideline is more restrictive for lower velocity movements. This contradiction can be attributed to the fact that even though the generic model was scaled to the participants of each simulation, the same RRA parameters were used for both the simulations. The gait focused RRA parameters in the OpenSim simulation reference likely worked better for gait compared to SLJL and produced lower residuals. The purpose of this section was only to show the implementation of our MATLAB function and it was not intended to investigate different RRA parameters.

These results, however, demonstrate that both the model and simulation parameters should be participant-specific to generate reasonable simulations through processes like RRA, especially for fast movements. One way to find participant-specific RRA parameters is the use of an outer-level optimization (Reinbolt et al., 2011), where an optimization routine optimizes the human-defined RRA parameters to reduce simulation residuals. This technique has been used by researchers to generate reasonable simulations of fast movements like side-cutting (Donnelly et al., 2012c) and SLJL (Gupta et al., 2018b) with negligible residuals. Researchers can also use this technique to reduce the residuals for satisfying the new guidelines, similar to our implementation of the outer-level optimization (Reinbolt et al., 2011) in this study.

2.5.3. Effect of different residual recommendations on simulation results

In the simulations that met the new guidelines, residual moment MY_p was the most restrictive because the residual MY_p directly affects ΔMY_{ZMP} unlike other residuals whose effect on $\Delta \bar{r}_{ZMP}$ and ΔMY_{ZMP} gets attenuated by dividing by the vertical experimental $\bar{F}_{GRF}$ (Eq. 2.7-2.9). Our analyses show that following different residual recommendations can result in different simulation results. The differences in kinetics suggest that a difference in muscle contributions could potentially be expected and lead to different conclusions for clinical interpretations of simulation-based studies.

2.6. Conclusion

In this study, we made new residual threshold guidelines that take into account the dynamic, physics-based characteristics of the movement. We demonstrated that the new guidelines are more restrictive than the original 2015 ones. Moreover, we showed that following different sets of recommendations can lead to different simulation kinetics, which may lead to different conclusions and clinical recommendations. We advocate the use of these new guidelines as they accept only those simulations considering the dynamic, physics-based characteristics of the movement. The new guidelines are the next step in the evolution of the residual threshold recommendations and, like Hicks et al. (2015), we believe that these guidelines will continue to evolve as researchers use simulation studies for more complex movements. There are several areas where this evolution may occur. When generating dynamic simulations, it is possible to have different simulated kinematics for the same externally applied forces and moments to reduce the residuals. Further research is necessary to investigate the addition of kinematics-based constraints to the new threshold guidelines. Since simulated kinetics were found to be different when meeting different sets of residual threshold recommendations, it is expected that the computed muscle activities may be different as well. Future work that investigates this effect would better the understanding of the relationship between residual reduction and muscle contributions to further refine the threshold guidelines.

2.7. Acknowledgement

We thank Caroline Finch, David Lloyd and Bruce Elliott for providing experimental data for the single-leg jump-landing movement (NHMRC grant: 400937).

CHAPTER THREE

STUDY II: OPTIMAL WHOLE-BODY KINEMATICS DURING SINGLE-LEG JUMP-LANDING TO REDUCE PEAK AB/AD- DUCTION AND INTERNAL ROTATION KNEE MOMENTS: IMPLICATIONS FOR ANTERIOR CRUCIATE LIGAMENT INJURY RISK

3.1. Abstract

Knee ab/ad-duction moment and knee internal rotation moment are known surrogate measures of anterior cruciate ligament (ACL) injury risk during tasks like sidestepping and single-leg landing. Previous experimental literature has shown that a variety of kinematic strategies are associated or correlated to ACL injury risk; however, the optimal kinematic strategies needed to reduce peak knee moments and ACL injury are not well understood. To understand the complex, multi-faceted kinematic factors underpinning ACL injury risk and to determine optimal kinematics strategies to prevent the ACL injury, a musculoskeletal modeling and simulation experimental design was used. A 14-segment, 37 degree-of-freedom, dynamically consistent skeletal model driven by force/torque actuators was used to simulate whole-body single-leg jump-landing (SLJL) kinematics. Using the residual reduction algorithm in OpenSim, optimal whole-body kinematics were generated that reduce the peak knee ab/ad-duction and int/ext rotation moments simultaneously. This optimization was repeated across 30 SLJL trials from 10 participants. The general optimal kinematic strategy was to bring the knee to a more neutral alignment. This was featured by reduced hip adduction angle and increased knee adduction angle. This optimal whole-body kinematic strategy significantly reduced peak knee ab/ad-duction and internal rotation moments, transferring most of the knee load to the hip.

3.2. Introduction

Approximately 200,000 anterior cruciate ligament (ACL) injuries are documented in the United States each year (Brophy et al., 2009; Utturkar et al., 2013). With surgical reconstructions considered best clinician treatment, coupled with long rehabilitation periods (4-12 months), ACL injuries cost the US health care system up to \$1.5 billion USD annually (Kramer, 2010). The effects of ACL injuries are also severe to the injured athlete as only 45% reach full recovery (Dunn and Spindler, 2010), with over half developing knee osteoarthritis within 10 years of their injury. With the majority of ACL injuries being non-contact in nature (Cochrane et al., 2007), many researchers and clinicians believe the most effective manner to reduce the burden of ACL injuries on society is through injury prevention (proactive) versus injury management (reactive) protocols.

ACL strain and injury risk is the greatest during the weight acceptance phase of the landing and sidestepping tasks (Brown et al., 2014b; Cerulli et al., 2003; Donnelly et al., 2012b). The ACL strain is elevated by anterior tibial forces in concert with ab/ad-duction and internal rotation knee moments (Besier et al., 2001; Chaudhari et al., 2005; Dempsey et al., 2007; Markolf et al., 1995; McLean et al., 2005). It is important to note that it is the combination of ab/ad-duction and internal rotation knee moments that elevates the ACL strain and injury risk more than either in isolation (Markolf et al., 1995). Therein, it should be the focus of injury prevention frameworks to reduce both ab/ad-duction and internal rotation moments during the weight acceptance phase of single-leg landing and

sidestepping if we are to effectively reduce ACL strain, injury risk, and injury incidence in society.

Researchers have investigated the effect different techniques and postural combinations can have on peak knee ab/ad-duction moments during sidestepping and landing. Knee ab/ad-duction moment has been correlated to sagittal (Donnelly et al., 2012c) and non-sagittal plane knee kinematics (Zazulak et al., 2007), knee range of motion (Myer et al., 2005), hip kinematics (McLean et al., 2005), foot strike posture (Donnelly et al., 2017; Stearne et al., 2014), trunk kinematics (Dempsey et al., 2007; Donnelly et al., 2012c; Zazulak et al., 2007), arm kinematics (Chaudhari et al., 2005), and balance control (Cochrane et al., 2010). These studies have helped establish associated links between different sporting techniques/postures, knee joint loading, and ACL injury risk; however the complexity and interconnectedness of the multifaceted system that is the human body has prevented researchers from making unified technique recommendations for reducing ACL injury risk in sport. To address this concern, Donnelly et al. (2012b) used optimization methods with computer simulations to find optimal whole-body kinematics during high velocity sporting tasks. They found that the general kinematic strategy to reduce the peak valgus knee moment during sidestepping task was to redirect the whole-body center of mass (COM) towards the desired direction of travel. The absence of a foot-contact model limits the interpretation and applicability of their results relating to the foot kinematics, which led to externally verify this finding using a different population and experiment

design (Donnelly et al., 2017). Another noted limitation was reducing only the ab/ad-duction knee moments without considering the internal rotation knee moment.

Building upon the computational framework developed by Donnelly et al. (2012b), the aim of this study was to identify optimal whole-body kinematics to reduce both ab/ad-duction and internal rotation moments simultaneously during weight acceptance phase of single-leg jump-landing (SLJL). To address the limitations identified by Donnelly et al. (2012b), we integrated zero moment point (ZMP) computations within the *in silico* framework, which is a computationally elegant way to generate dynamically-consistent ground reaction forces (GRFs) during the weight acceptance phase of SLJL (Reinbolt and Donnelly, 2017b; Xiang et al., 2010).

3.3. Methods

We used experimental data from a pool of previously collected research data (Dempsey et al., 2012; Donnelly et al., 2012c; Morgan et al., 2014). The experimental data simulations were built from a pool of 34 amateur male Australian Rules Football players performing an established SLJL protocol. From this data, 10 participants were randomly selected for this study (height 1.87 ± 0.06 m; mass 85.6 ± 8.5 kg; age 21.8 ± 4.0 years). Ethical approval for this data collection was obtained from the Human Research Ethics Office at the University of Western Australia (RA/4/1/5713).

All participants performed a variety of SLJL trials using their preferred leg (right for the 10 selected participants) for both take-off and landing. For all the trials, the participants were asked to run into the calibrated motion capture volume at 4.5-5 m/s and jump to a height of 90% their maximum vertical jump height and mark (or grab) an Australian Rules football (Dempsey et al., 2012). Participants were exposed to both non-perturbed and perturbed jump-landing trials. During the perturbed jump-landing trials, the Australian Rules football was swung away to either their left (perturbation left trials) or their right (perturbation right trials). During the non-perturbed jump-landing trials (no perturbation trials), the football was not swung away from the participants. All trials were performed in random order and the participants were not told if, and in what direction the ball will move. During all jump-landing trials, participants landed on a 1.2 m x 1.2 m force plate (AMTI Inc., Watertown, USA) recording at 2,000 Hz. A 12 camera, Vicon MX system (VICON, Oxford, UK) was used to record motion data at 250 Hz with a UWA Full Body Model (Dempsey et al., 2012). Both kinematic and GRF data were low pass filtered at 15 Hz using a 4th order zero-lag Butterworth filter.

A 14 segment, 37 degree of freedom, force/torque actuated model formed the foundation of all 30 SLJL simulations (Donnelly et al., 2012c). Subtalar and metatarsophalangeal (mtp) joints were locked to reduce computational complexity in the subsequent motion optimization. Participant-specific models were created by scaling the segment lengths based on experimentally derived joint center positions. Segment inertial properties were scaled to each participant's total body

mass in OpenSim 3.3 (SimTK.org)(Delp et al., 2007). Inverse kinematics was performed using the experimental marker data to generate generalized coordinates for each trial of all the participants ($n = 30$).

This was followed by a 2-step optimization process. The first step serves to reduce simulation residuals to generate an optimal model that accurately represents the experimental data. Residual forces and moments of an inverse dynamic solution represent the errors between the net dynamics of a musculoskeletal model and the experimental ground reaction force measures (i.e., criterion measure). The residual reduction algorithm (RRA) in OpenSim is a computational approach to minimize the simulation's residual forces and moments by adjusting the center of mass of the trunk segment and simulation kinematics. Similar to Donnelly et al. (2012b), we used an outer-level optimization(Reinbolt et al., 2011) to find optimal parameters of model used by inner level optimization which was the RRA optimization. These parameters are the 37 maximal force/torque of the force/torque actuators (R^{max} and T^{max}) and the 37 weights at which the kinematics are tracked in the cost function of RRA ($w_{\ddot{q}}$). To address the lack of a foot contact model, we integrated ZMP computations in the outer-level optimization routine. ZMP computations predict the GRFs based on the simulation kinematics (Reinbolt and Donnelly, 2017b; Xiang et al., 2010). We added the error between the ZMP predicted GRF and the experimental GRF to the cost function of the outer-level optimization. This technique generated simulations with near zero residuals and dynamically-consistent GRF, and provided an optimal mass-

adjusted model with optimal kinematic-tracking weights and optimal maximum capacity of the force/torque actuators. Similar to Donnelly et al. (2012b), a simulation was accepted if the residuals were near zero, kinematic translation error < 3 cm, kinematic rotational error < 5°, GRF force error < 10 N, free-moment error < 10 Nm and center of press (COP) error < 3 cm.

Step 1 inner-level optimization cost function:

$$\min_{x^R, x^T} \left[\sum_{i=1}^{n_q} w_{\ddot{q}_i} (\ddot{q}_i^{exp} - \ddot{q}_i^{sim})^2 + \sum_{j=1}^6 \left(\frac{R_j(x_j^R)}{R_j^{max}} \right)^2 + \sum_{k=1}^{n_T} \left(\frac{T_k(x_k^T)}{T_k^{max}} \right)^2 \right] \quad (3.1)$$

Where, x^R and x^T are the excitation levels (control magnitude) of the force and torque actuators. $\ddot{q}^{exp}$ and $\ddot{q}^{sim}$ are the experimental and simulation generated accelerations and $w_{\ddot{q}}$ are the tracking weight of the n_q degrees of freedom. R are the 6 residuals (three forces and three torques). T are the torques generated by the $n_T = n_q - 6$ torque generators. R^{max} and T^{max} are maximum possible values for residuals and joint torques, respectively.

Step 1 outer-level optimization cost function:

$$\min_{w_{\ddot{q}}, R^{max}, T^{max}} \sum_{i=1}^{n_f} \left[W_{pelvis} \sum_{j=1}^6 (q_{ij}^{exp} - q_{ij}^{sim})^2 + W_{non-pelvis} \sum_{j=7}^{n_q} (q_{ij}^{exp} - q_{ij}^{sim})^2 \right. \\ \left. + W_R \sum_{k=1}^6 R_{ik}^2 + W_{GRF} \sum_{m=1}^6 (GRF_{im}^{exp} - GRF_{im}^{ZMP})^2 \right] \quad (3.2)$$

The outer-level minimizes the error between the n_q experiment (q^{exp}) and simulation (q^{sim}) kinematics, the 6 residuals (R), and the error between 6 GRF quantities from experimental GRF (GRF^{exp}) compared to ZMP-computed GRF (GRF^{ZMP}). These quantities are minimized over the entire weight acceptance phase (frame $i = 1$ to n_f). This cost function has multiple terms that are governed

my non-linear dynamic constraints making this a non-linear multi-objective problem. Additionally, each term is features squared terms. The 74 design variables make this a large problem from the point of view of simulation generation because each iteration of the outer-level cost function runs the entire simulation generating algorithm of inner level optimization (RRA). For this reason, we used gradient-based non-linear least square optimization algorithm for the outer-level optimization. Once an optimal model, kinematics tracking weights, and maximum actuators forces/torques were generated for a participant using a randomly selected trial, they were not changed for the rest of the trials of that participant. For each participant, the trial with the highest vector sum of ab/ad-duction and int/ext rotation knee moments in each of the three types of trials (no perturbation, perturbation left and perturbation right) was selected for step 2 of optimization that finds the optimal whole-body kinematics to reduce the risk of ACL injury. These selected trials put the participant at increased risk of ACL injury compared with other trials.

Step 2 of optimization was another outer-level optimization routine (Reinbolt et al., 2011). To simultaneously reduce the ab/ad-duction and internal rotation knee moments, the penalty of using these torque actuators ($T_{V/V}$ and $T_{I/E}$) was increased in the RRA optimization by a factor ($f_{V/V}$) and ($f_{I/E}$), respectively. At the same time, to allow the kinematics to change, most kinematic tracking weights were reduced by a factor ($f_{\ddot{q}}$). The pelvis tracking was not reduced since its movement affects the ZMP, which can in-turn affect the dynamic consistency of

the model by forcing the COP outside of the foot. The outer-level optimization design variables $f_{\ddot{q}}$, $f_{V/V}$, and $f_{I/E}$ were adjusted to minimize the vector sum of ab/ad-duction and int/ext rotation knee moments during the weight acceptance phase. A simulation was not accepted if the ZMP did not stay under the foot. Hence, the ZMP computations ensure dynamic consistency by ensuring that the effective COP of the new movement (its zero-moment point) stays within the base of support (the foot). This optimization resulted in a novel simulation with optimal whole-body kinematics with reduced vector sum of ab/ad-duction and int/ext rotation knee moments.

Step 2 inner-level optimization cost function:

$$\min_{x^R, x^T} \left[\sum_{i=1}^6 w_{\ddot{q}_i} (\ddot{q}_i^{exp} - \ddot{q}_i^{sim})^2 + \sum_{i=7}^{n_q} f_{\ddot{q}} w_{\ddot{q}_i} (\ddot{q}_i^{exp} - \ddot{q}_i^{sim})^2 + \sum_{j=1}^6 \left(\frac{R_j(x_j^R)}{R_j^{max}} \right)^2 + \left(\frac{T_{V/V}(x_{V/V}^T)}{f_{V/V} T_{V/V}^{max}} \right)^2 + \left(\frac{T_{I/E}(x_{I/E}^T)}{f_{I/E} T_{I/E}^{max}} \right)^2 + \sum_{k=1}^{n_T-2} \left(\frac{T_k(x_k^T)}{T_k^{max}} \right)^2 \right] \quad (3.3)$$

Step 2 outer-level optimization cost function:

$$\min_{f_{\ddot{q}}, f_{V/V}, f_{I/E}} \sum_{i=1}^{n_f} \left[T_{V/V}^2 + T_{I/E}^2 \right] \quad (3.4)$$

Where, the outer-level finds optimal factors $f_{\ddot{q}}$, $f_{V/V}$, and $f_{I/E}$. These factors are multiplied by the parameters $w_{\ddot{q}}$, $T_{V/V}^{max}$ and $T_{I/E}^{max}$ determined by the step 1 optimization process. We used gradient-based non-linear least square optimization algorithm for the outer-level optimization again since this was still a non-linear multi objective problem.

Using the same methods as Donnelly et al. (2012b), we computed “critical coordinates” that changed following the optimization by more than 2 standard

deviations above the mean change of all coordinates. Since the kinematic changes were the result of minimizing the vector sum of ab/ad-duction and int/ext rotation knee moments, these critical coordinates represent the most influential coordinates to reduce these knee moments. All data processing, calls to OpenSim 3.3 simulation tools, and optimization was performed using MATLAB (R2017a, MathWorks Inc, Natick, Massachusetts, USA). For statistical analyses, a two-way repeated measures ANOVA was used with the three perturbation conditions as the first factor and pre-or-post optimization as the second factor ($\alpha = 0.05$). All statistical analyses were performed using SPSS (IBM Corp. IBM SPSS Statistics for Windows, Version 25.0, Armonk, NY, USA).

3.4. Results

Pre-to-post optimization, there was a significant reduction in the vector sum of ab/ad-duction and int/ext rotation knee moments ($60 \pm 14 \%$). These reductions were attributed to significant reductions in peak adduction moment (Fig. 3.1.c), abduction moment (Fig. 3.1.c) and internal rotation moment (Fig. 3.1.e). Interestingly, there were significant increases in peak hip abduction moment pre-to-post optimization. Peak sagittal plane moments for the hip, knee and ankle did not increase pre-to-post optimization (Fig. 3.1.a-b). These simulated optimal whole-body kinematics had near zero residual forces and moments along with dynamically consistent GRF.

There were nine critical joint coordinates across 30 simulations that most influenced the reduction of the vector sum of ab/ad-duction and int/ext rotation

knee moments following the optimizations (Table 3.1). The following five of these nine coordinates were consistently critical, that is, critical in more than a half of the simulations: 1) the knee adduction angle, 2) knee internal rotation angle, 3) hip adduction angle, 4) hip internal rotation angle, and 5) frontal plane trunk angle. The knee adduction angle and the hip abduction angle increased pre-to-post optimizations (Table 3.1). Additionally, these angle changes progressively increased from perturbation left to no perturbation to perturbation right trial conditions. Similarly, progressively higher increases in knee internal rotation angle was observed pre-to-post optimization from perturbation left to no perturbation to perturbation right trial condition (Table 3.1).

3.5. Discussion

Ab/ad-duction and internal rotation knee moments are known surrogate measures of ACL injury risk during sporting tasks like sidestepping and SLJL. Our group and others have investigated the effects of movement modification to reducing these moments. In this study, we integrated the ZMP computations (Reinbolt and Donnelly, 2017b; Xiang et al., 2010) to extend the previous computational modeling and simulation framework (Reinbolt et al., 2011) addressing the limitation of the absence of a foot contact model in the previous simulation study on ACL injury (Donnelly et al., 2012c). We used this extended framework to determine optimal whole-body kinematics for the weight acceptance phase of the SLJL. The peak ab/ad-duction and peak internal rotation knee moments reduced significantly pre-to-post optimization across the perturbation

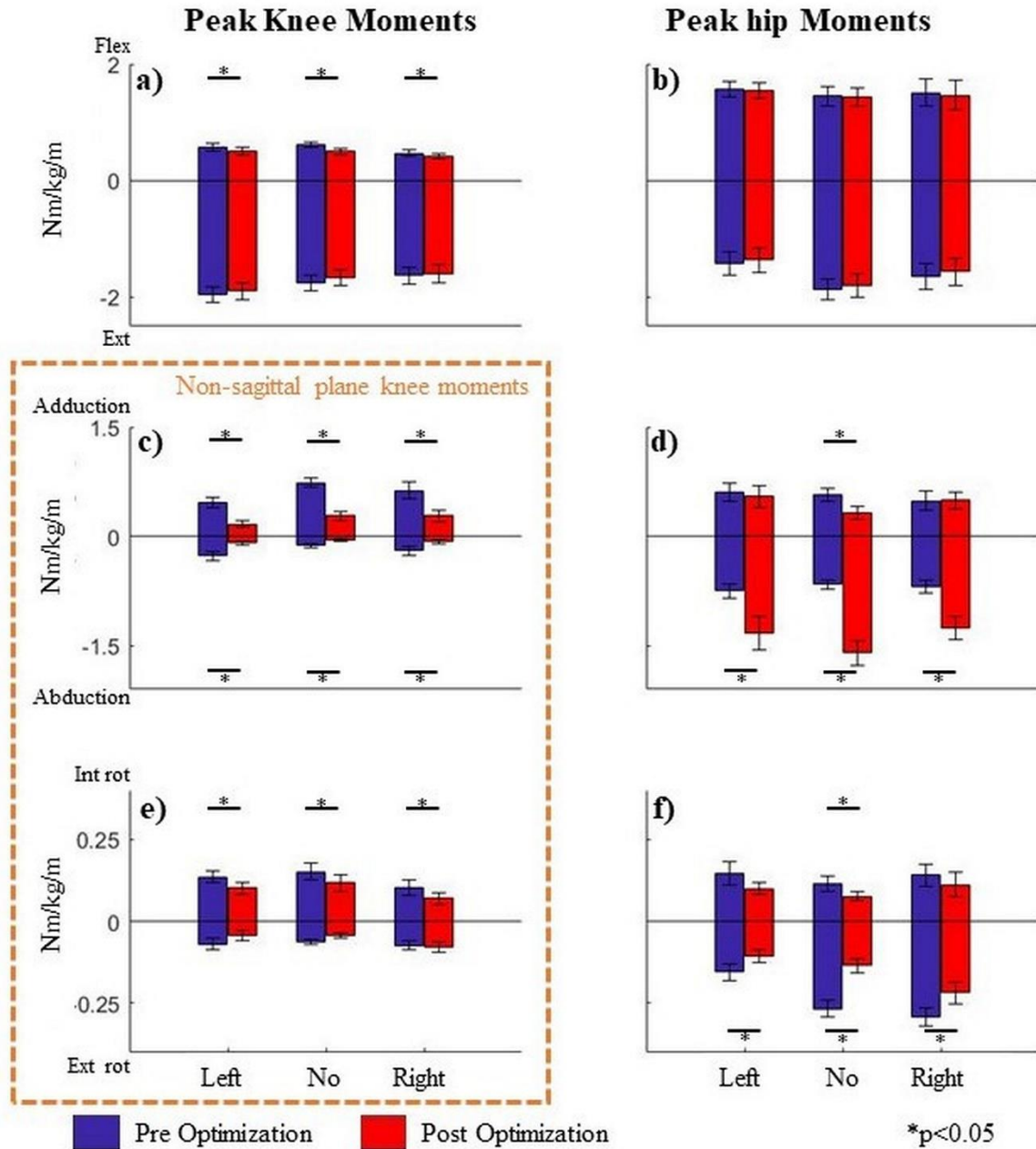


Figure 3.1. Mean $\pm$ standard error values of peak moments pre and post optimization of knee and hip of stance leg, normalized to body mass and body height. Pre-to-post optimization, the peak knee abduction/adduction moment (3.1.c) and peak knee internal rotation moment (3.1.e) decreased significantly, while the peak hip abduction moment (3.1.d) increased significantly.

Table 3.1. All critical coordinates and the mean change in their value pre-to-post optimization.

Coordinates critical in at least half of the simulations (consistently critical coordinates) are bolded.

Perturbation	Consistently Critical (critical for at least half of the simulations)					Ankle Dorsi- flexion Stance Leg	Hip Adduction Swing Leg	Lumbar Rotation (transverse plane)	Hip Flexion Stance Leg
	Hip Adduction Stance Leg	Knee Adduction Stance Leg	Lumbar Lateral Flexion (frontal plane)	Hip Internal Rotation Stance Leg	Knee Internal Rotation Stance Leg				
Left	-1.18	1.11	0.51	-0.87	-0.18	-	-0.64	0.62	-1.04
No	-1.78	2.41	0.75	-0.37	1.13	-1.64	-0.53	0.61	0.59
Right	-2.15	3.35	0.63	1.18	2.14	-	-0.22	1.92	-

conditions, which helps reduce the ACL strain (Markolf et al., 1995). It was also observed that the knee ab/ad-duction moment was the bigger contributor to the non-sagittal plane knee moment compared to the knee int/ext moment (Fig. 1.c & 1.e) with peak knee adduction moment being on average 4.7 times larger than peak knee internal rotation moment, across the perturbation conditions. It is still important to reduce the knee internal rotation moment along with the knee ab/ad-duction knee moment since the knee internal rotation moment has more deleterious effects on the ACL compared to the knee ab/ad-duction moment (Markolf et al., 1995). At the same time, we observed that the peak hip abduction moment increased significantly across all perturbation conditions (Fig. 1.d) suggesting that majority of the knee loads transferred to the hip which is better equipped to handle the higher load because of the higher degree of freedom and the musculature surrounding the hip joint.

Pre-to-post optimization, we found that nine coordinates were critical to influencing the reduction of dangerous knee moments, out of which five were consistent (Table 1). Unlike Donnelly et al. (2012b), we found all critical coordinates were from the lower body or trunk. We also found that unlike Donnelly et al. (2012b), there was minimal to no changes in the sagittal plane pre-to-post optimization. There were no consistent critical coordinates identified in the sagittal plane. Reduction in the ACL injury related knee loads has been associated with increased flexion angle of the stance limb (Donnelly et al., 2012c) to promote a fore-foot landing compared to a rear-foot landing. Experimental studies

(Chinnasee et al., 2018; Donnelly et al., 2017) have also confirmed that fore-foot landing reduces loads on the knee and is better to prevent ACL injury compared to rear-foot landing. We still did not observe changes in the sagittal plane kinematics pre-to-post optimization. This is because SLJL is typically fore-foot and all trials in this study had a fore-foot landing pattern. Hence, the sagittal plane kinematics for our data may have already been optimal to reduce knee loads associated with ACL injury.

Interestingly, we observed that even though we reduced the vector sum of ab/ad-duction and int/ext rotation knee moments, the peak external rotation knee moment did not reduce significantly (Fig. 3.1.e). This finding, however, does not affect the implications of our results since the ACL strain is not dependent on high external rotation knee moments (Markolf et al., 1995). We also observed that pre-to-post optimization the peak knee flexion moments reduced significantly, and the peak knee extension moment also reduced (Fig. 3.1.a). This finding, along with the absence of changes in knee flexion angle pre-to-post optimization, ensures that our optimal kinematics do not deleteriously push the knee in the sagittal plane, but rather transfer the knee loads to other segments of the body, sparing the knee that is at a high risk of injury during the landing task.

Our study has a few limitations. First, we locked the subtalar joint and the metatarsophalangeal (mtp) joints to neutral positions to reduce the computational complexity for our optimizations. The subtalar joint can potentially help reduce the knee ab/d-duction moment by reducing the length of the lever arm that the GRF

makes about the knee. Second, due to the computational complexity, we only included data from 10 participants, one trial in each perturbation conditions. Third, we weighted the knee ab/d-duction moment and the knee int/ext rotation moment equally in the cost function of the outer-level optimization in step 2. Since the knee ab/d-duction moments are typically higher than the knee int/ext rotation moments, this would result in simulations that favor reduction of knee ab/d-duction moments more than the knee int/ext rotation moments. Fourth, residuals represent external forces or moments and since we reduced the residuals in step 2 of the study the kinematics changed pre-to-post optimization but the change to the center of mass trajectory was near zero. Nonetheless, we were still able to find optimal whole-body kinematics that would reduce both knee ab/d-duction and knee internal rotation moments simultaneously.

To better understand the mechanism of reduction of the ab/ad-duction knee moments, we studied the length of the lever arm that the GRF vector makes with the knee in the frontal plane. Figure 2 displays the results of table 3.1, such that the mechanism of reduction of ab/ad-duction and internal rotation knee moments could be observed. Fig. 3.2.d shows the minimal length of this lever arm, normalized to the participant's height, pre-to-post optimization across the three perturbation conditions. We found that the optimization framework was able to reduce the peak knee ab/ad-duction moment by reducing the lever arm of the GRF about the knee in the frontal plane (Fig. 3.2.a-d). Based on the changes in kinematics (Table 3.1), we can infer that the reduction in lever was achieved by

increasing the knee adduction angle and the hip abduction angle pre-to-post optimization (Fig. 3.2.d). Mechanically, this significantly reduced the peak knee ab/ad-duction moments (Fig. 3.1.b) and increased the peak hip abduction moments (Fig. 3.1.e) across all three perturbation conditions pre-to-post optimization. This indicates that the high knee ab/ad-duction moments get transferred to the hip, which is better equipped to handle the higher load because of the higher degree of freedom and the musculature surrounding the hip joint.

Additionally, we observed that the lever arm was progressively increased from perturbation left trials to no perturbation trials to perturbation right trials pre optimization. This explains the progressively higher increase in knee adduction angle and hip abduction angle observed from perturbation left to no perturbation to perturbation right condition pre-to-post optimization (Table 3.1). Kinematically, this resulted in a reduction of knee ab/ad-duction angle to near zero post optimization (Fig. 3.2.e). Similarly, we also found that post optimization, the knee int/ext rotation angle became closer to zero (Fig. 3.2.f). Anatomically, both knee ab/ad-duction and knee int/ext rotation angles being near zero would reduce the ACL strain by bringing the knee to a neutral position in both the frontal and transverse plane, reducing the risk of ACL injury.

Our results may have major implications in the field of preventive medicine. Through our *in silico* study we were able to identify the cause and a potential correction mechanism for preventing ACL injury. These results may help develop and enhance biomechanically-informed training to prevent ACL injury during SLJL

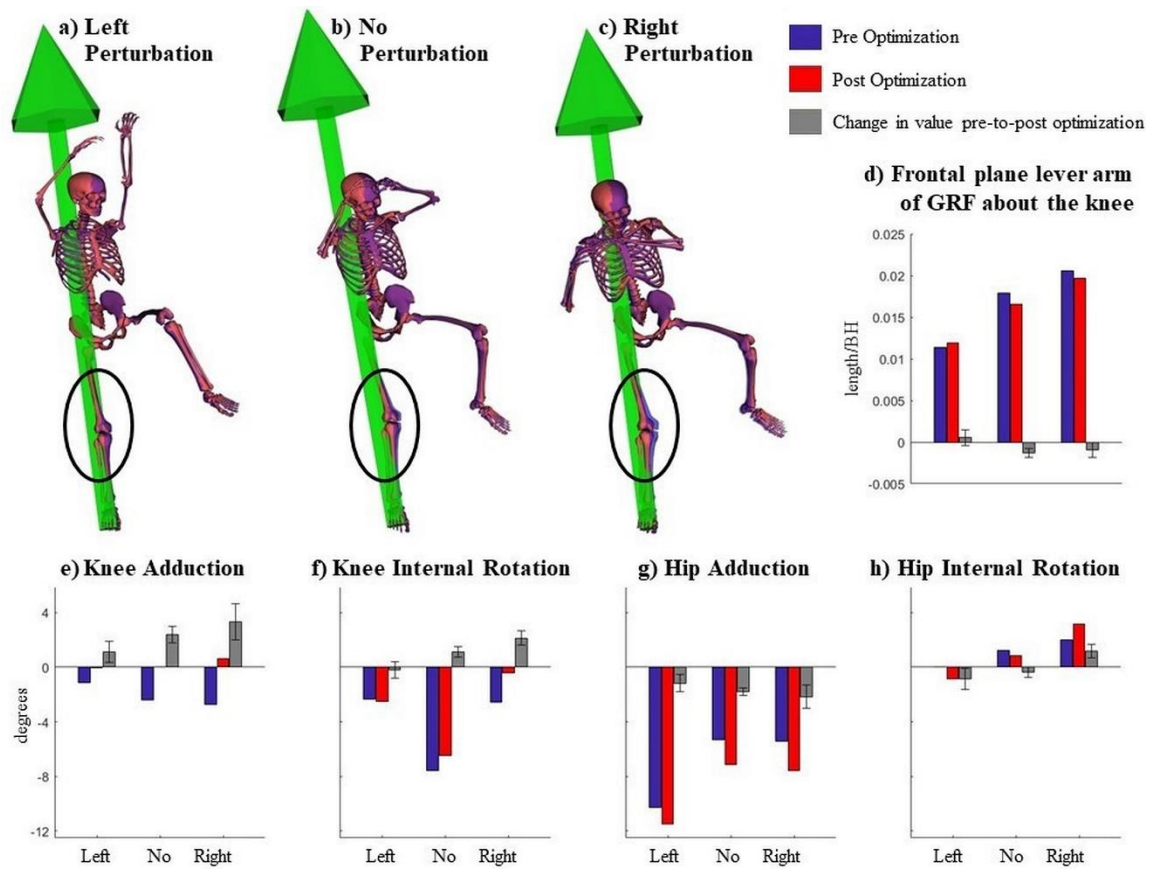


Figure 3.2. Mechanism of reduction of non-sagittal plane knee moments. Snapshots of perturbation left (**3.2.a**), no perturbation (**3.2.b**) and perturbation right (**3.2.c**) for a participant. The knee gets placed closer to the ground reaction force vector, especially in no perturbation (**3.2.b**) and perturbation right (**3.2.c**) for this participant. Mean value and mean $\pm$ standard error change in value of: **3.2.d** Frontal plane lever arm of ground reaction force about the knee (normalized to body height) and **3.2.e-h** Consistently critical coordinates of lower limbs as shown in Table 1. Pre-to-post optimization, the knee abduction/adduction angle (**3.2.e**) and knee internal/external rotation angle (**3.2.f**) became closer to zero.

(Donnelly et al., 2020). For example, based on the current study, an instruction like “increase your hip abduction” during SLJL could be simple and achievable goal for athletes to prevent the ACL injury. We recommend an experimental study with a larger participant pool to test our *in silico* result and the external validity.

3.6. Acknowledgement

We thank Caroline Finch, David Lloyd and Bruce Elliott for providing experimental data (NHMRC grant: 400937). This work was supported in part by the National Science Foundation (CAREER #1253317).

CHAPTER FOUR

STUDY III: USE OF GOAL-ORIENTED OPTIMIZATION OF DYNAMIC SIMULATIONS TO FIND A BALANCE BETWEEN PERFORMANCE AND INJURY PREVENTION DURING VOLLEYBALL SPIKING

4.1. Abstract

Performance enhancement (i.e., peak height and forward velocity of the hitting hand) and injury prevention (i.e., shoulder injuries) are two pillars supporting long-term success in any sport. These aspects are often perceived as two opposite sides of a coin, where if one focuses on one, it is to the detriment of the other. For the volleyball spiking motion, the peak height of the hitting hand and its forward velocity are two important performance parameters. The most common site of injury during volleyball spiking is the shoulder. It is primarily caused by high mechanical loads applied across the shoulder joint, which are most pronounced during the follow-through phase of the movement. In this study, we used physics-based simulations to model participant-specific whole-body mechanics of the volleyball spiking motion. We used volleyball spiking data from 13 skilled individual volleyball athletes. There were 104 trials for the power phase and 209 trials for the follow-through phase. Our simulations increased ($p < 0.05$) the peak height of the hitting wrist by 1% (performance), increased ($p < 0.05$) the forward wrist velocity by 25% (performance), without increasing peak shoulder joint torques (injury risk). Our simulations also reduced ($p < 0.05$) shoulder joint torques by 75% during the follow-through phase. Our results indicate that the primary mechanism to increase performance parameters was to elevate the forward swing of the lower limbs (i.e., hip flexion, knee extension), and the primary mechanism to reduce torques across the shoulder joint during follow-through was the synergistic rotation of the trunk

along the pathway of the hitting arm. Our results demonstrate that performance and injury prevention are not mutually exclusive.

4.2. Introduction

Optimizing performance without increasing an athlete's injury risk during arm swing phase of a volleyball spike are two pillars supporting the long-term success of a volleyball attacker. The height of the hitting hand and its forward velocity are important determinants of performance during the power phase of this motion, while the most common site of injury during this motion is the shoulder joint during the follow-through phase (i.e., eccentric loading) (Briner and Kacmar, 1997; Eerkes, 2012; Wang and Cochrane, 2001). A balance between optimal performance and injury risk during this motion is considered a difficult training task as optimal performance in this task is coupled with high velocities and accelerations, the same variables that are known to underpin musculoskeletal injuries (Donnelly et al., 2012a). The balance between performance and injury prevention is something that coaches and athletes strive to achieve, but rarely accomplished when using a heuristic or intuitive experimental approach. Kinematics changes non-linearly affect both performance (Brown et al., 2014a; Seminati et al., 2015; Serrien et al., 2016) and shoulder injury risk (James et al., 2014; Leonard and Hutchinson, 2010; Mihata et al., 2010; Seminati et al., 2015; Shih and Wang, 2019) during a volleyball spiking motion. For this reason, identifying optimal kinematic patterns can achieve optimal performance while not

increasing shoulder injury risk (Seminati et al., 2015). The downstream effects for this method to advance the field of athletic training and rehabilitation is paramount.

High magnitude and high frequency loads applied to the shoulder during the spiking motion is a known risk factor related to overhead hitting shoulder injuries (Challoumas et al., 2017; Eerkes, 2012; Kugler et al., 1996; Lajtai et al., 2012; Reeser et al., 2010). Because of the complexity of the shoulder joint, an injury to this joint and surrounding soft tissues can manifest in many ways. These include but are not limited to rotator cuff muscle/tendon injury (Briner and Kacmar, 1997; Leong et al., 2017; Wang and Cochrane, 2001), suprascapular neuropathy (Dramis and Pimpalnerkar, 2005; Igielska-Bela et al., 2020), and impingement injuries (Mirhassan Zadeh Kuhkamar et al., 2020). The major cause of injury during the volleyball spiking motion is believed to be high eccentric stress on the relatively smaller rotator cuff muscles which are used as “breaks” to decelerate the fast-moving arm during the follow-through phase of the spike motion (Briner and Kacmar, 1997; Wang and Cochrane, 2001). Hence, a reduced eccentric mechanical load on the shoulder can potentially reduce the risk of shoulder injury during volleyball spiking.

Modified kinematics have been proposed in the literature that can potentially reduce the risk of injury and enhance performance at the same time. Seminati et al. (2015) compared the traditional spiking style to an alternate hitting style, known as the backswing style, which is arguably generic or non-specified in nature. They found that the alternate style resulted in a potentially safer path of humeral rotation,

while increasing ball velocity. This study, however, did not measure or predict the forces and torques applied across the shoulder during either the power or follow-through phase. Additionally, it is difficult to fit an athlete's movement to a generic technique. It can be argued the technique should be tailored to the athlete, thus invalidating the practical applicability of this study in a real-world setting. Other kinematic variables like hip angular velocity (Brown et al., 2014a) and orientation of trunk and pelvis (Serrien et al., 2016) have been related to performance. Kinematics like humeral and scapular range of motion (Mihata et al., 2010; Shih and Wang, 2019) and humeral rotation velocity (Seminati et al., 2015) have been associated with shoulder injury. Although these studies help understand various aspects of injury and performance, they are limited in scope since they do not encompass the kinematics or kinetics of the whole body meaning they do not characterize the entire kinematic and kinetic chain of the hitting motion. It has been shown that optimal movement of body segments far from the injury cite can reduce loads on the primary injury cite (Donnelly et al., 2012c).

Musculoskeletal modeling of the whole-body combined with simulation allows us to ask “what if” questions, which are difficult, time intensive, and costly to answer with a heuristic experimental approach (Delp et al., 2007; Dembia et al., 2019). This is because it is very difficult to test and study interconnected influences of all segments along the kinematic and kinetic chain and their influence on specific biomechanical parameters like the forces and torques applied across the shoulder; or performance parameters like the height and velocity of the hitting hand of a

volleyball player. Optimization methods with musculoskeletal modeling and computer simulations have been used to find optimal whole-body kinematics during high velocity sporting tasks to reduce the risk of injury (Donnelly et al., 2012c; Gupta et al., 2018a; Gupta et al., 2019b; Gupta et al., 2018b), but never to our knowledge to enhance sporting performance.

In this study, we used novel methods to achieve a performance-injury prevention balance. Since typical simulation-generating methods depend on tracking a given trajectory by solving for excitation of torque actuators, the joint loads represented by the activation of the actuators can be controlled. However, it is hard to find a new kinematics that meets performance goals since it would imply tracking kinematics that we essentially want to find creating a chicken-or-egg kind of problem. To solve this problem, we employed a novel technique of generating a hypothetical target trajectory of the performance segment that depicts a large increase in the performance parameters, to the extent that might not even be anatomically and dynamically feasible. Tracking this hypothetical trajectory with appropriate weights pushes the trajectory of the performance segment of the simulation towards the hypothetical target trajectory. This can force a change in all segments of the body, but since the system is still subject to anatomical and dynamic constraints, the resulting kinematics will depict a higher performance while still being feasible. Additionally, we added goal-oriented terms in the cost function of the optimization process, a novel way of designing optimization cost functions in the simulation literature. These terms increase the efficiency of the

optimization process to generate simulations that can achieve both a desired performance goal and an injury prevention goal by introducing step functions in the overall cost function. These terms also make the optimization process capable of handling specific performance or injury related goals that coaches or athletes may present with, making this method more robust and adaptable.

In this study, we used the optimal dynamic simulation generation process to find participant-specific optimal whole-body kinematics for volleyball spiking that enhances performance and reduces shoulder injury risk simultaneously. To increase performance during the power phase (when the elbow starts to go forward following maximum cocking until the last frame before ball contact (McConnell et al., 2011)), we focused on increasing the peak height of the hitting hand and its forward velocity at peak height. At the same time, we ensured that the peak shoulder torques did not increase, thus mitigating or maintaining injury risk during the power phase. To reduce the risk of shoulder injury during the follow-through phase (the first frame after ball contact until 30 ms after the peak shoulder torques), where eccentric forces are at their highest (Briner and Kacmar, 1997; Eerkes, 2012; Wang and Cochrane, 2001), we focused on reducing the peak shoulder joint torques. Note that increasing the performance parameters during power phase can increase the humeral angular velocity during the power phase, which can cause injury in the follow-through phase. Additionally, increasing performance parameters while mitigating shoulder loads during the power phase can increase loads on other joints of the body, putting them at a risk of injury. Similarly, reducing

loads on the shoulder during the follow-through phase when rapid deceleration of the arm is required can add loads on other joints along the kinematic and kinetic chain. For these reasons, we did not allow increases in peak humeral angular velocity and restricted the allowable increase in joint torques across all joints. During the optimization process, we ensured that the optimized motion was not too different from the original motion, increasing the likelihood that the optimal motions can be learned, increasing the practical applicability of our results. The null hypothesis tested in this study is that there will be no significant increases in performance pre-to-post optimization in the power phase. We also tested the null hypothesis that there will be no significant differences in joint torques pre-to-post optimization in the follow-through phase.

4.3. Methods

4.3.1. Experimental data

We used data from a pool of data collected for a previous study (Gupta et al., 2021). This is a dataset of spiking motion of 15 skilled volleyball hitters collected in a motion capture laboratory using a 10 MX camera Vicon motion capture system (Vicon Motion Systems, Oxford, UK). The athletes hit the ball in three different conditions: 1) natural hitting, 2) maximal knee flexion in mid-flight and 3) no knee flexion in mid-flight. In total, 209 trials were used for simulation purposes in the power phase and 249 in the follow-through phase. The lab was set up to resemble game conditions as much as possible, with the net set at the standard height, center line, 3m attack line, and the ball placed at their preferred hitting height.

Ethical approval for the data collection was obtained from the Institutional Review Board of The University of Texas at Austin (Study 2014-09-0072). All participants used for this study contacted the ball with their right hand (7 men, 6 women).

4.3.2. Musculoskeletal model

We used a force/torque actuated upper and lower body musculoskeletal model (simtk.org). This model combines the generic lower limbs and trunk model (Delp et al., 2007; Delp et al., 1990) with the upper extremity model (Holzbaur et al., 2005). For computational efficiency, we locked the subtalar and metatarsophalangeal (mtp) joints and removed the spline function in the knee flexion angle. Additionally, we locked the wrist joints since there was only one marker on the hand. The model had 29 degrees of freedom, six for the pelvis, five for each leg (three for the hip, one for the knee, and one for the ankle), three for the trunk and five for each arm (three for the shoulder, one for elbow flexion, and one for pronation supination). This generic model was scaled to each participant in OpenSim 3.3 (Delp et al., 2007). Inverse kinematics was performed to generate the generalized coordinates for each spiking trial. The three shoulder coordinates, consistent with the ISB recommendations are shown in Fig 4.1.

4.3.3. Two-step optimization process

Inverse kinematics was followed by a two-step optimization process, similar to the one described by Donnelly et al. (2012), to find optimal whole-body kinematics. Each step of this process is an outer-level optimization (Reinbolt et al., 2011). Outer-level optimization is an optimization routine that is used to optimize

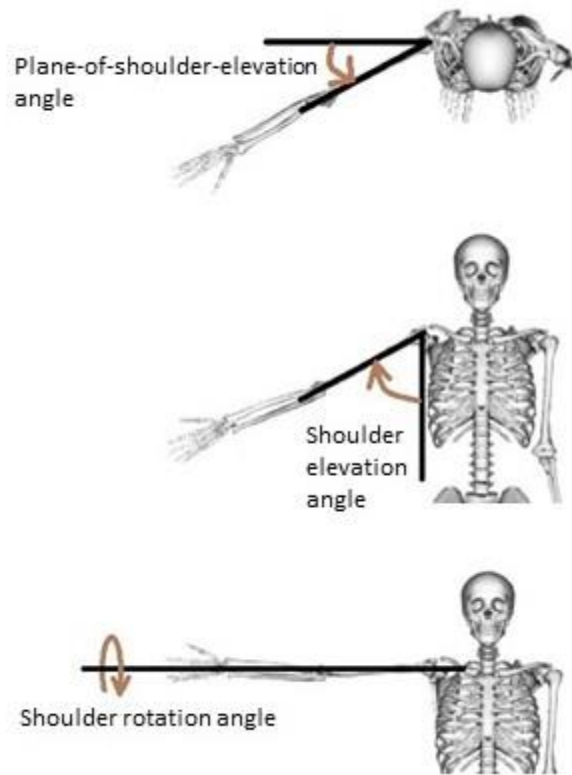


Figure 4.1: Depiction of the shoulder coordinates

the parameters of the simulation generated by the inner level optimization process; for this study, the residual reduction algorithm (RRA) in OpenSim was used. Hence, each cost function evaluation of the outer-level optimization is a new simulation. Fig. 4.2 depicts the two-step optimization process described below. Simulations were not time-normalized before RRA since RRA performs a computation every millisecond, which should be kept constant for all athletes.

4.3.3.1. Step 1 of optimization process

The first outer-level optimization ensures that the experimental data is accurately represented in the simulations by optimizing the human-defined parameters of the model to reduce simulation residuals (Donnelly et al., 2012c; Gupta et al., 2019b; Reinbolt et al., 2011). These parameters are the 29 maximal force/torque capacity of actuators (R^{max} and T^{max}) and the 29 weights at which the joint coordinates are tracked by the cost function of the RRA ($w_{\ddot{q}}$).

Step 1 RRA cost function:

$$\min_{x^R, x^T} \left[\sum_{i=1}^{n_q} w_{\ddot{q}_i} (\ddot{q}_i^{exp} - \ddot{q}_i^{sim})^2 + \sum_{j=1}^6 \left(\frac{R_j(x_j^R)}{R_j^{max}} \right)^2 + \sum_{k=1}^{n_T} \left(\frac{T_k(x_k^T)}{T_k^{max}} \right)^2 \right] \quad (4.1)$$

Where, x^R and x^T are the excitation of the force and torque actuators. $\ddot{q}^{exp}$ and $\ddot{q}^{sim}$ are the experimental and simulation-generated accelerations, $w_{\ddot{q}}$ are the tracking weights of the $n_q = 29$ degrees of freedom, R are the six residuals (three forces and three torques), T are the torques generated by the $n_T = n_q - 6$ torque actuators, and R^{max} and T^{max} are the maximum capacity of the residuals and joint torque actuators, respectively. The outer-level optimization optimizes

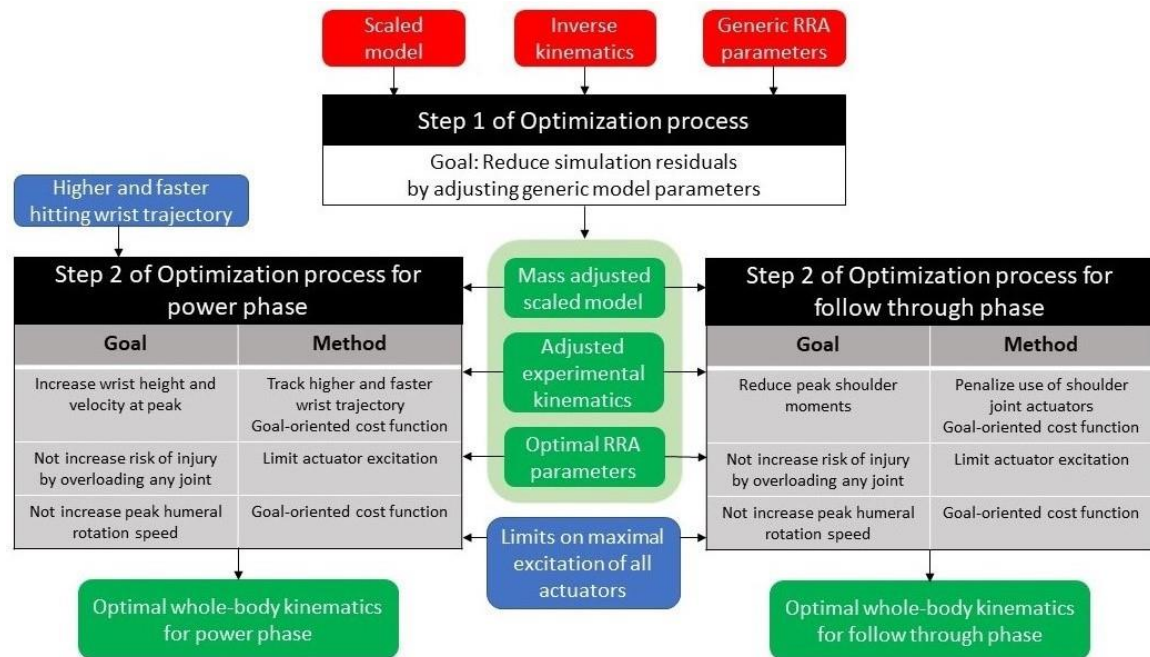


Figure 4.2: The two-step optimization process to find optimal whole-body kinematics.

parameters of the RRA optimization to ensure that the simulation kinematics (q^{sim}) are dynamically consistent with the experimental kinematics (q^{exp}) and that the residuals (R) are near zero.

Step 1 outer-level optimization cost function:

$$\min_{w_{\dot{q}, R}^{max}, T^{max}} \sum_{i=1}^{n_f} \left[\begin{aligned} &W_{pelvis} \sum_{j=1}^6 (q_{ij}^{exp} - q_{ij}^{sim})^2 \\ &+ W_{non-pelvis} \sum_{j=7}^{n_q} (q_{ij}^{exp} - q_{ij}^{sim})^2 + W_R \sum_{k=1}^6 R_{lk}^2 \end{aligned} \right] \quad (4.2)$$

Where, $W_{pelvis} = 500$, $W_{non-pelvis} = 1000$ and $W_R = 1000$ were manually chosen weights of the terms in the cost functions and n_f is the number of frames over which the optimization was performed. The optimization was performed from the start of the forward motion of the elbow to hit the ball and lasted until 30 ms after the peak shoulder torques in the follow-through phase. Since RRA uses 1 ms time steps when generating a simulation, we found that 30 ms was sufficient to capture peak shoulder torques during the follow-through phase of the simulation. This process gives us a mass adjusted participant-specific scaled model, participant-specific RRA parameters, and adjusted experimental kinematics. The kinematics are adjusted to be dynamically consistent and reduce pelvis residuals, which represent the errors and assumptions made in the modeling process (Donnelly et al., 2012c; Reinbolt et al., 2011). Once we obtained optimal model parameters for each participant using the first outer-level optimization, these calculated parameters were kept constant for all trials of the same participant. We accepted the simulations only if the absolute value of average residual forces < 1N, absolute value of average residual moments < 5 Nm, kinematic translation

error < 3 cm, and kinematic rotational error < 5°. The same error parameters have been used in previous studies (Donnelly et al., 2012c; Gupta et al., 2019b; Gupta et al., 2018b). Since the outer-level optimization is required to handle a large number of design variables, we used gradient-based optimization for this process.

4.3.3.2. Step 2 of optimization process

Once optimal, participant-specific model parameters were obtained in the step 1 of optimization process, they were used again for the second step optimization. For step 2 of optimization process (or the second outer-level optimization), the goal of the optimization is to optimize the dynamics of the model to satisfy a performance or injury-related goal such as elevating hand velocity and height and/or reducing or maintaining peak joint torques. The power phase of overhead hitting involves both performance enhancement and injury prevention aspects, while the follow-through phase concentrates on injury prevention aspects. As the goal of the optimization changed between the power phase and the follow-through phase, step 2 of optimization procedures was performed in parts, then interpreted together within the analysis section.

4.3.3.2.1. Step 2 of optimization process for power phase

The goal of this optimization is to find optimal whole-body kinematics that enhances performance without increasing the risk of injury. This entails satisfying two performance goals and three injury prevention goals simultaneously. The performance goals are: 1) increase the peak height of the hitting wrist, and 2) increase the forward velocity of the hitting wrist at its peak. The injury prevention

goals are: 1) prevent peak shoulder torques from increasing, 2) prevent overload of any other joint torque in the whole-body kinetic, and 3) do not allow peak humeral angular velocity magnitude (HAVM) to increase. To ensure that we do not overload any joint, a limit on the maximal allowable excitations was applied on each joint coordinate's actuator. This limit represents the peak torque of that joint coordinate actuator in that trial plus one standard deviation of peak torque of that coordinate across all trials in that gender and hitting condition, during the power phase. For the three coordinate actuators of the shoulder joint, this limit was their peak torque in that trial since we did not want to increase the peak shoulder torques. To ensure that the peak HAVM does not increase while the performance parameters increase, we used a goal-oriented cost function for the outer-level optimization.

Humeral angular velocity magnitude (HAVM) is the vector sum of the velocities of the three shoulder coordinates. To ensure that the optimization does not increase the peak HAVM, we added a goal-oriented term in the cost function of the outer-level optimization to account for it.

$$HAVM \text{ term} = \begin{cases} peak \ HAVM, & peak \ HAVM > peak \ HAVM_{exp} \\ 0, & otherwise \end{cases} \quad (4.3)$$

Where *peak HAVM* is the peak HAVM of the simulations generated during the outer optimization process and *peak HAVM_{exp}* is the peak HAVM of the experimental kinematics. This goal-oriented cost functions mean that for the simulations generated during the optimization process, if the peak HAVM exceeds the experimental peak HAVM, the *HAVM term* takes the value of the *peak HAVM*.

Otherwise, it takes a value of 0. This step function in the outer-level optimizer cost function encourages the optimization to favor the simulations that do not allow an increase in the peak HAVM pre-to-post optimization.

Similarly, goal-oriented cost function terms were added to promote an increase in the peak height of the hitting wrist and the forward velocity of the hitting wrist at its peak height. We calculated the percent increase in the peak height of wrist (pIH), the percent increase in the forward velocity of the wrist at its peak height (pIV), and designed a wrist cost function term.

$$Wrist\ term = \begin{cases} (pIH \times pIV) + 10, & pIH < 0 \text{ and } pIV < 0 \\ -(pIH \times pIV) - 10, & pIH > 0 \text{ and } pIV > 0 \\ pIH \times pIV, & \text{otherwise} \end{cases} \quad (4.4)$$

Using a product of pIH and pIV in the cost function ensures that the outer-level optimization does not favor either increase in peak height or velocity over the other. The ± 10 part of the wrist term encourages the optimizer to favor simulations which increase both peak height and velocity at peak height of the wrist, simultaneously. At the same time, this wrist term ensures that the optimization does not favor the simulations that decrease either or both performance parameters.

The final cost function of the outer-level optimization, that is, the step 2 outer-level optimization cost function for power phase is a weighted sum of the HAVM term and the wrist term.

$$Cost\ function = W_{HAVM} \times HAVM\ term + W_w \times Wrist\ term \quad (4.5)$$

Where, $W_{HAVM} = 0.005$ and $W_w = 0.1$ were manually chosen. Since the terms of the cost function have step functions in them, gradient-based optimization cannot be used for the outer-level optimization. We used the simulated annealing algorithm (Goffe et al., 1994) because it can handle non gradient-based cost functions, and it is a global optimization algorithm as opposed to a local one.

In addition to the terms in the outer-level cost function, the simulation generating process (RRA) controlled by the outer-level needs to be able to find new motions that meet the performance and injury prevention goals. To allow the RRA to find a new optimized motion, tracking weights of all upper limb coordinates, lower limb coordinates and trunk rotation about the vertical axis were reduced by a factor. This factor was one of the design variables of the outer-level optimization that controls the inner level RRA. The tracking of the pelvis coordinates was not reduced since pelvis movement directly affects residuals. Additionally, trunk and pelvis vertical excursion affects hang-time of the volleyball athletes (Gupta et al., 2015; Gupta et al., 2021). Hang-time is a period of time when the athlete is around the peak of his/her flight, and the head and trunk of the athlete seems to stay at a constant vertical height (Bishop and Hay, 1979). Studies have shown that athletes tend to swing later when they use hang-time, increasing their decision-making time before ball contact, which can potentially enhance performance (Fortin-Guichard et al., 2020; Gupta et al., 2021). For this reason, we did not want to change the hang-time of the volleyball athletes, and hence we did not reduce the tracking of the coordinates that influence hang-time.

To promote the RRA to find motions that increase the peak height of the hitting wrist and its forward velocity, we added a tracking task in the cost function of the RRA. This tracking task penalized the difference between the trajectory of the hitting wrist and a hypothetical target trajectory that was $p\%$ higher and $v\%$ faster than the experimental trajectory of the hitting wrist. The values of p and v were design variables of the outer-level optimization. The power phase begins when the elbow starts to move forward, and it is unreasonable to increase the height and forward velocity of the hitting wrist at the start of power phase. Hence, the target trajectory was designed such that the increase in height was maximal at the peak ($p\%$) and zero at the lowest point of the experimental trajectory of the hitting wrist. At each time frame i , an increase in height of the target trajectory compared to the experimental trajectory is $(x_{pi} \times p)\%$, where $x_{pi} = \frac{\text{height at frame } i - \min \text{ height}}{\text{max height} - \min \text{ height}}$. The same implementation was used for the forward velocity increase as well. At each time frame i , the increase in forward velocity of the target trajectory compared to the experimental trajectory is $(x_{vi} \times v)\%$, where $x_{vi} = \frac{\text{forward velocity at frame } i - \min \text{ forward velocity}}{\text{max forward velocity} - \min \text{ forward velocity}}$. Fig. 4.3 shows an example of the experimental and the target trajectory.

Step 2 RRA cost function for follow-through phase:

$$\min_{x^R, x^T} \left[\sum_{i=1}^8 w_{\ddot{q}_i} (\ddot{q}_i^{exp} - \ddot{q}_i^{sim})^2 + \sum_{i=9}^{n_q} f_{\ddot{q}} w_{\ddot{q}_i} (\ddot{q}_i^{exp} - \ddot{q}_i^{sim})^2 + \sum_{j=1}^6 \left(\frac{R_j(x_j^R)}{R_j^{max}} \right)^2 \right. \\ \left. + \sum_{k=1}^{n_T} \left(\frac{T_k(x_k^T)}{T_k^{max}} \right)^2 + w_p (Y_{WJC}^{tgt} - Y_{WJC}^{sim})^2 + w_v (X_{WJC}^{tgt} - X_{WJC}^{sim})^2 \right] \quad (4.6)$$

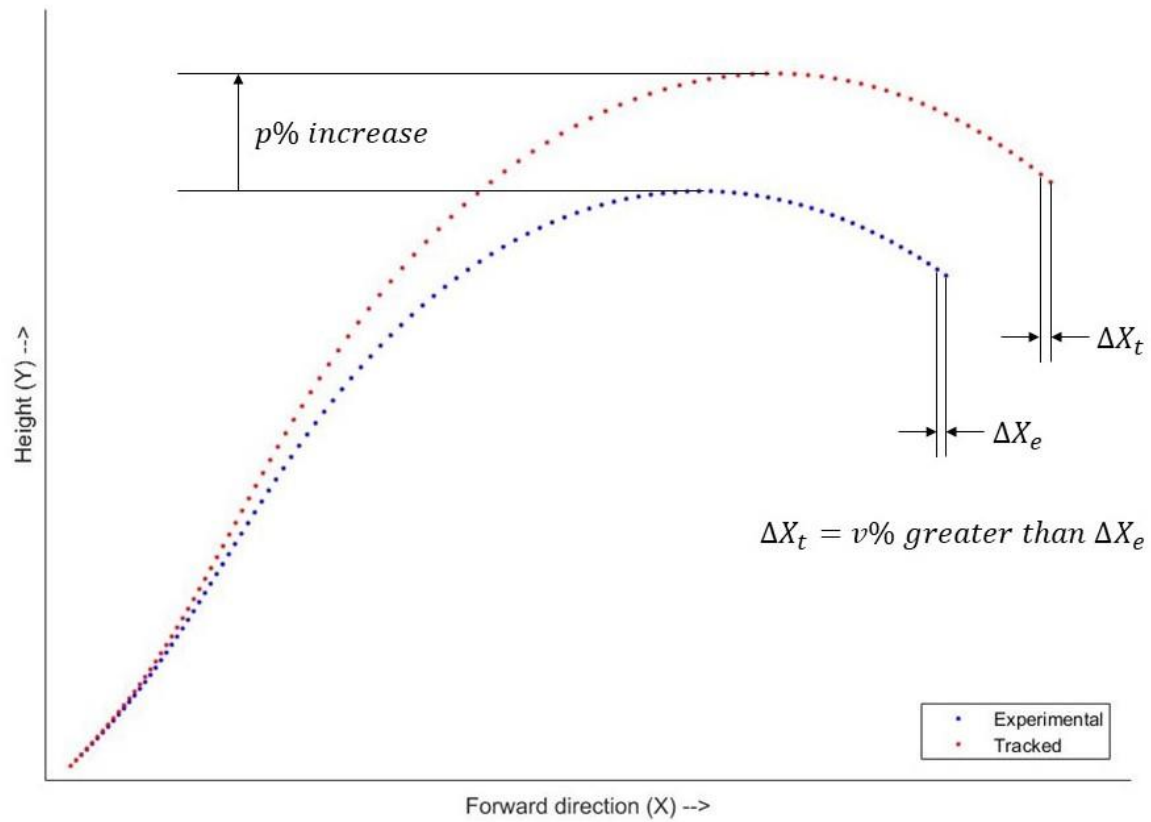


Figure 4.3. Sagittal plane view of experimental and target trajectory of the wrist joint center of the hitting arm. Each marker represents a time frame. Both trajectories have the same lowest point and lowest forward velocity. The peak of the target trajectory is $p\%$ higher than that of the experimental trajectory. The experimental trajectory usually recorded its highest forward velocity just before ball contact, or the last frame of the power phase. At the last frame, the forward velocity (difference between forward position of consecutive frames) of the target trajectory is $v\%$ greater than that of the experimental trajectory.

Where, $k = 1$ to 8 are for the six pelvis and two trunk coordinates whose tracking weights are not reduced, tracking weights of all other coordinates are reduced by a factor $f_{\ddot{q}}$. The weights $w_p = 1000$ and $w_v = 1000$ were manually chosen. The last two terms of the cost function represent the difference between the X and Y positions of the simulation hitting wrist joint center (X_{WJC}^{sim} and Y_{WJC}^{sim}) and those of the target trajectory of the hitting wrist joint center (X_{WJC}^{tgt} and Y_{WJC}^{tgt}). This trajectory is $p\%$ higher and $v\%$ faster than the experimental trajectory of the hitting wrist. $f_{\ddot{q}}, p$ and v are the design variables of the outer-level optimization. Again, optimal values of $w_{\ddot{q}}, R^{max}$ and T^{max} were determined in step 1 of the optimization process.

Even though the goal-oriented cost function terms encourage the cost function to generate simulations of specific biomechanical properties, it is possible that it fails. For example, it is possible that a simulation achieves an extremely high percent increase in the forward velocity at peak height (say $pIV = 20$) by reducing the peak height (say $pIH = -1$). This scenario will lead to a value of -20 for the *Wrist term* (Eq. 4.4). The optimizer will prefer this to a 1 percent increase in both peak height and forward velocity, which leads to a value of -11 for the *Wrist term* (Eq. 4.4). On the other hand, it is also possible that the even though residual reduction is a part of the cost function, the simulation still generates high residuals if it reduces the cost from other terms. To address this such issues, we accepted a post optimization simulation only if it met all the following acceptance criteria a) increased peak height of the hitting wrist, b) increased forward velocity at peak

height of the hitting wrist, c) decreased peak HAVM, and d) absolute value of the average residual forces and residual moments are lower than 5 N and 5 Nm, respectively.

4.3.3.2.2. Step 2 of optimization process for follow-through phase

The goal of this optimization is to find optimal whole-body kinematics that reduces peak external rotation joint torques and risk of shoulder injury. This entails satisfying three injury prevention goals simultaneously. These goals are: 1) reduce peak shoulder torques, 2) prevent overloading of any other joint of the body and 3) prevent peak HAVM from increasing. Similar to the power phase, to ensure that we do not overload any joint other than the shoulder, we restricted the torque production of each coordinate actuator to not exceed the peak torque of that coordinate actuator in that trial plus one standard deviation of peak torque of that coordinate across all trials in that sex and hitting condition, during the follow-through phase. Additionally, we used the same HAVM term in the outer-level cost function as the one used in the power phase outer-level cost function to ensure that the peak HAVM did not increase pre-to-post optimization. To reduce the peak torques of the shoulder joint coordinates in the follow-through phase, we designed a new goal-oriented cost function term, the shoulder torque (ST) term, one for each direction (positive and negative) of each of the three shoulder coordinates.

For the i^{th} shoulder coordinate, the ST term in j^{th} direction is:

$$ST\ term_{ij} = \begin{cases} rM_{ij} + 1, & rM_{ij} > 0.9 \\ rM_{ij}, & otherwise \end{cases} \quad (4.7)$$

Where, rM_{ij} is the ratio of the peak shoulder torque in the j^{th} direction of the i^{th} shoulder coordinate to the experimental peak shoulder torque of that coordinate ($i = 1,2,3$ and $j = 1,2$). This implementation encourages the optimization to favor simulations that allow for at least 10% reduction in both peak positive and peak negative torques across each of the three shoulder coordinates.

The final step 2 outer-level optimization cost function for the follow-through phase was a weighted sum of the HAVM term and the ST terms.

$$Cost\ function = W_{HAVM} \times HAVM\ term + W_{ST} \sum_{i=1}^3 \sum_{j=1}^2 ST\ term_{ij} \quad (4.8)$$

Where, $W_{HAVM} = 0.01$ and $W_{ST} = 1$ were manually chosen. As in the power phase, the terms of the cost function of outer-level optimization in the follow-through phase have step functions in them. Hence, we again used simulated annealing algorithm for the outer-level optimization.

As in the power phase, we reduced the tracking weights of all coordinates, except the pelvis coordinates by a factor between 0 to 1. This factor was a design variable of the outer-level optimization. To ensure that the RRA reduced the peak shoulder torques, the penalty of using the torque actuators of the three shoulder coordinates was increased by a factor. Each coordinate was assigned a factor and these factors were also design variables of the outer-level optimization.

Step 2 RRA cost function for follow-through phase:

$$\min_{x^R, x^T} \left[\sum_{i=1}^6 w_{\ddot{q}_i} (\ddot{q}_i^{exp} - \ddot{q}_i^{sim})^2 + \sum_{i=7}^{n_q} f_{\ddot{q}} w_{\ddot{q}_i} (\ddot{q}_i^{exp} - \ddot{q}_i^{sim})^2 + \sum_{j=1}^6 \left(\frac{R_j(x_j^R)}{R_j^{max}} \right)^2 \right. \\ \left. + \sum_{k=1}^3 \left(\frac{T_k(x_k^T)}{f_k T_k^{max}} \right)^2 + \sum_{k=4}^{n_T} \left(\frac{T_k(x_k^T)}{T_k^{max}} \right)^2 \right] \quad (4.9)$$

Where, $k = 1,2,3$ are the three shoulder coordinates. $f_{\dot{q}}, f_1, f_2$ and f_3 are design variables of the outer-level optimization. Optimal values of $w_{\dot{q}}, R^{max}$, and T^{max} were determined in the step 1 of the optimization process.

Similar to the power phase, a post optimization simulation was accepted only if it met all the following acceptance criteria: a) all six ST terms were less than 0.9, implying that both peak positive and peak negative torques across all three shoulder coordinates reduced by at least 10%, b) decreased peak HAVM, and c) the absolute value of average the residual forces and residual moments are lower than 5 N and 5 Nm, respectively.

4.3.4. Post-hoc analyses

For both the power and follow-through phases of volleyball spiking, we wished to find the joint coordinates that elicited the changes in the hitting arm motion, ultimately causing changes in performance or shoulder injury risk parameters, which are termed critical joint coordinates (Donnelly et al., 2012c). Critical joint coordinates are those other than the hitting arm that changed more than two standard deviations above the mean change of all coordinates for each trial. Since each participant had multiple trials, we also computed the “consistent critical coordinates”. These were operationally defined as the joint coordinates that were critical for at least 40% of the trials of each individual participant. This helped us find participant-specific optimal kinematic changes that the simulation process chose to optimize the hitting motion. To understand the general pattern of kinematic changes that elicited the change in performance and injury prevention

parameters, we also computed the coordinates that were consistently critical for at least 40% of the participants. Similar methods were used in other computational biomechanics studies such as that described in chapter 3. All computations were performed using MATLAB (R2017a, The MathWorks Inc., Natick, MA, 2000) at the Texas Advanced Computing Center (TACC) at The University of Texas at Austin.

To compare changes in performance and injury prevention parameters in the power and follow-through phases, we compared the peak HAVM and the peak torques of the shoulder coordinates pre-to-post optimization. All torque values were normalized to body mass and body height. For the power phase, we also compared the peak height of the hitting wrist and the forward velocity at its peak height pre-to-post optimization. We used Hierarchical Linear Modeling (HLM) as the statistics tool, with participants as level 2 units and pre-vs-post optimization as level 1 variables ($\alpha = 0.05$). HLM removes the variance accounted by the level 2 units and focuses on differences in the variables of interest caused solely due to the level 1 variables, the optimization process. In other words, variance in the data due to participant-specific differences like height, weight, hitting position, age, experience, etc. are treated as covariates and their influence removed, thus allowing us to analyze the variance only due to the optimization procedure (Gupta et al., 2021; Staynor et al., 2019). All statistical tests were performed in R 3.3.1 (R Core Team, 2016, R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. URL <https://www.R-project.org/>).

4.4. Results

For the power phase (104 accepted trials), the mean peak height of the hitting wrist significantly increased ($p < 0.05$) by 1%. The mean forward velocity of the hitting wrist at its peak height significantly increased ($p < 0.05$) by 25%. Peak HAVM decreased ($p < 0.05$) pre-to-post optimization (Fig. 4.4. a.). At the same time, none of the peak torques at the shoulder increased pre-to-post optimization (Fig. 4.4. a.). Seven critical joint coordinates for at least 40% of the participants contributed to the observed changes in performance (Fig. 4.4.b.). The general kinematic change that elicit the changes in performance and injury-prevention parameters was the forward swinging of the legs that features increased hip flexion and knee extension. Supplementary data 4.1 gives a visual representation of the forward swing of the legs. Fig. 4.5 shows the consistent critical coordinates for all participants for the power phase. All participants seem to follow the general pattern of forward swing of the legs, at least to some extent.

For the follow-through phase (209 accepted trials), mean peak joint torques at the shoulder coordinates significantly decreased ($p < 0.05$). The mean peak HAVM reduced pre-to-post optimization. However, this decrease was not significant (Fig. 4.6. a.). The mean decreases in the range of torques across plane-of-shoulder-elevation angle, shoulder elevation angle and shoulder rotation angle coordinates were 80%, 88% and 56% (average 75%), respectively. Five critical coordinates across at least 40% of the participants were observed (Fig. 4.6. b.). These results suggest that the trunk rotates with the hitting arm to reduce the

Changes in power phase mechanics pre-to-post optimization

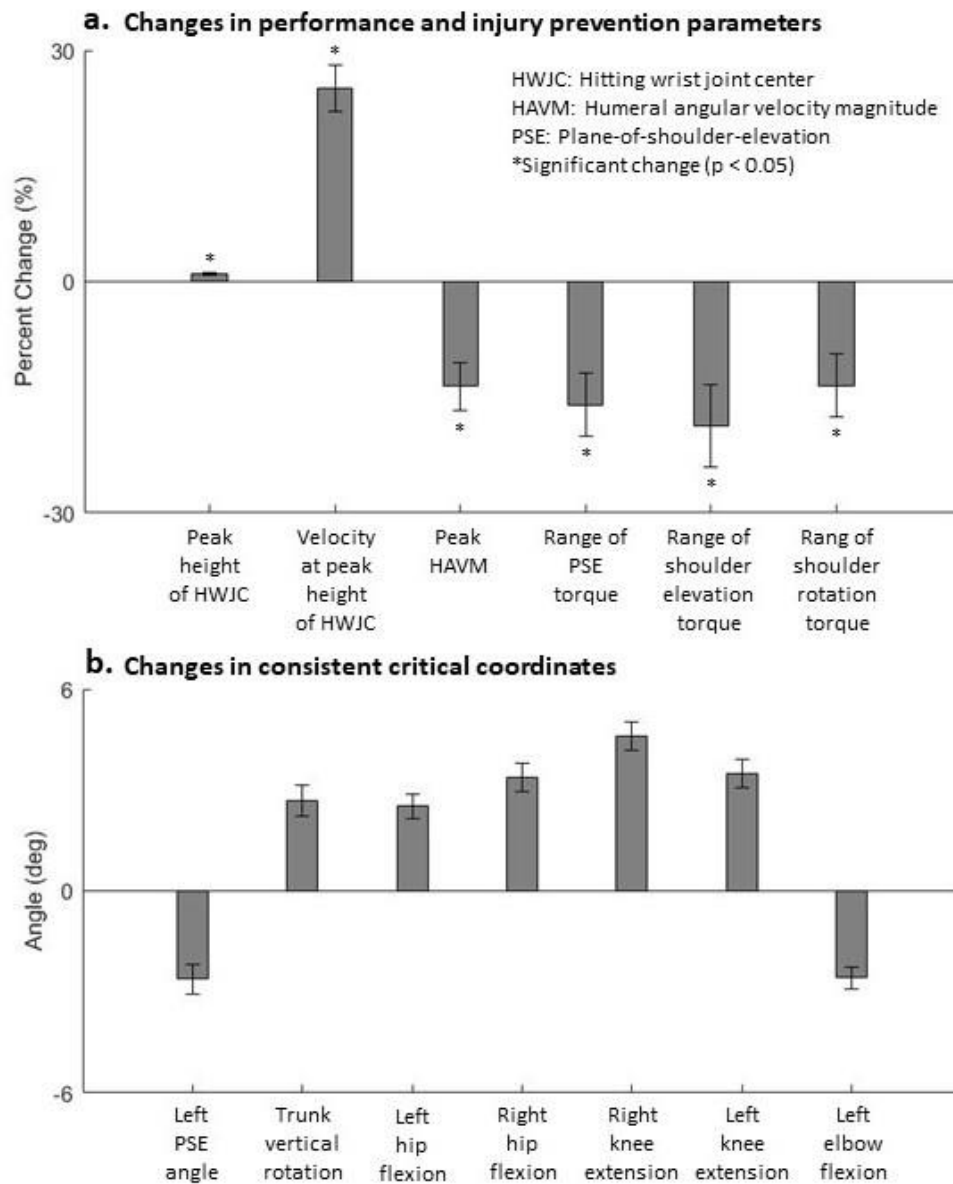


Figure 4.4. Changes in power phase pre-to-post optimization. **4.4.a.** Change in performance and injury prevention parameters. Mean $\pm$ standard error values across all participants are depicted. Note that in the statistical analyses, hierarchical linear modeling effectively compares trials of each participant pre-to-post optimization independent of other participants, rather than comparing all trials of all participants pre-to-post optimization. **4.4.b.** Coordinates that were consistently critical for at least 40% of the participants. These coordinates represent a general pattern that elicit the changes in performance and injury prevention parameters.

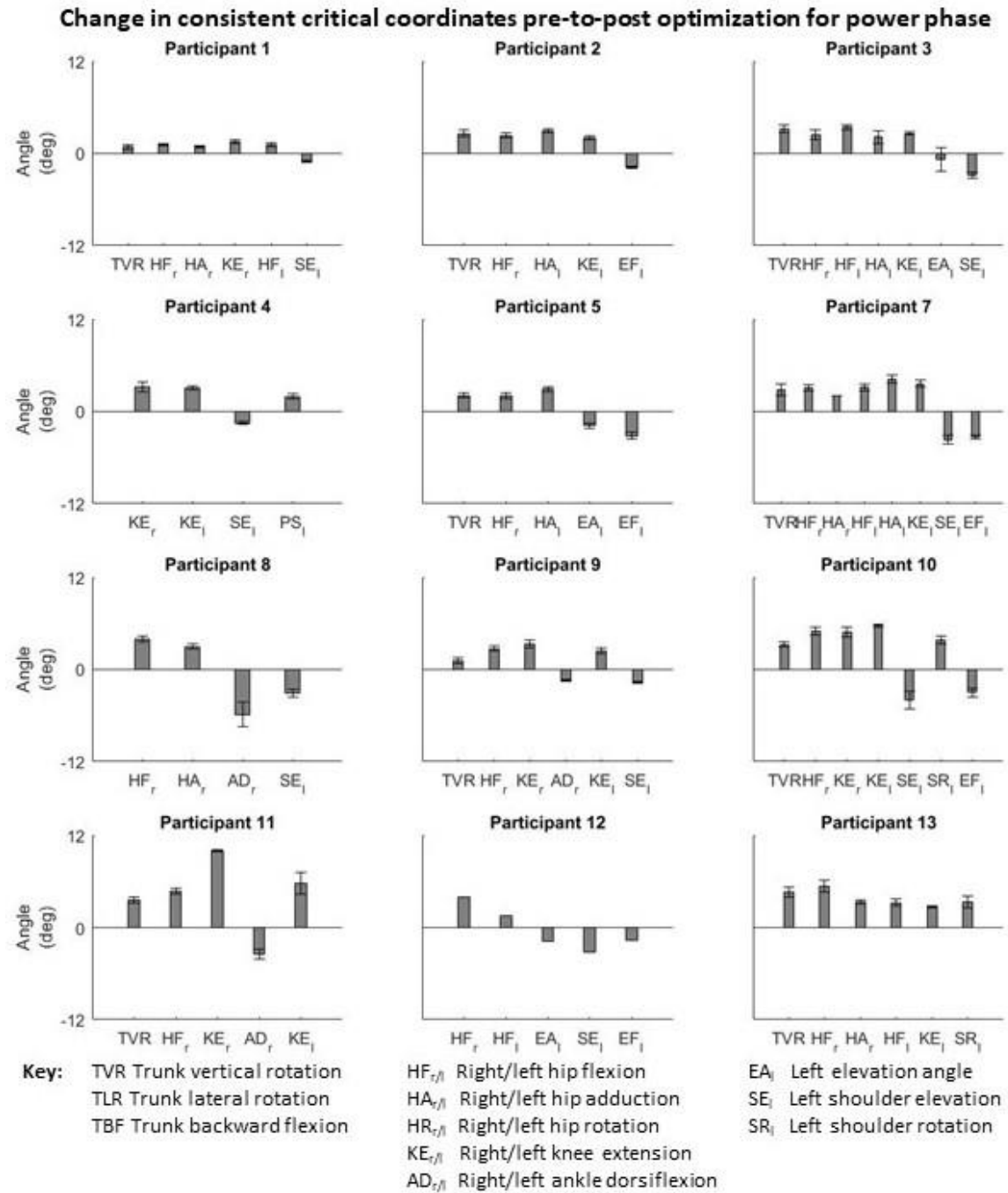


Figure 4.5. Consistent critical coordinates for all the participants during power phase.

torques at the shoulder. Supplementary data 4.2 provides a visual representation of this general pattern of the trunk following the pathway of the hitting arm. Fig. 4.7 shows the critical coordinates for all participants for the follow-through phase.

4.5. Discussion

In this study, we used the optimal dynamic simulation generation process to find optimal participant-specific, whole-body kinematic patterns during volleyball spiking that improved performance, without increasing injury risk at the shoulder or any other joint along the kinetic chain. These findings rejected our null hypothesis that the performance and injury prevention parameters will not change pre-to-post optimization. We found the key critical joint coordinates (called consistent critical coordinates), at both the participant level (Fig. 4.5 & 4.7) and the group level (Fig. 4.4 & 4.6), that elicited the changes in performance and injury prevention parameters for the power phase and the follow-through phase of the hitting motions. These include hip flexion and knee extension for the power phase and trunk vertical rotation for the follow-through phase. We can then recommend that athletes, coaches, and clinicians focus on these consistent critical coordinates during training and rehabilitation in efforts to learn optimal movement patterns that have the potential to enhance performance without increasing their risk of shoulder injury. Additionally, these results demonstrate that performance enhancement and injury prevention are not mutually exclusive, highlighting the utility of simulation for exploratory “what if” type research questions for clinical and athletic application.

Our goal-oriented optimization process grants athletes and coaches the

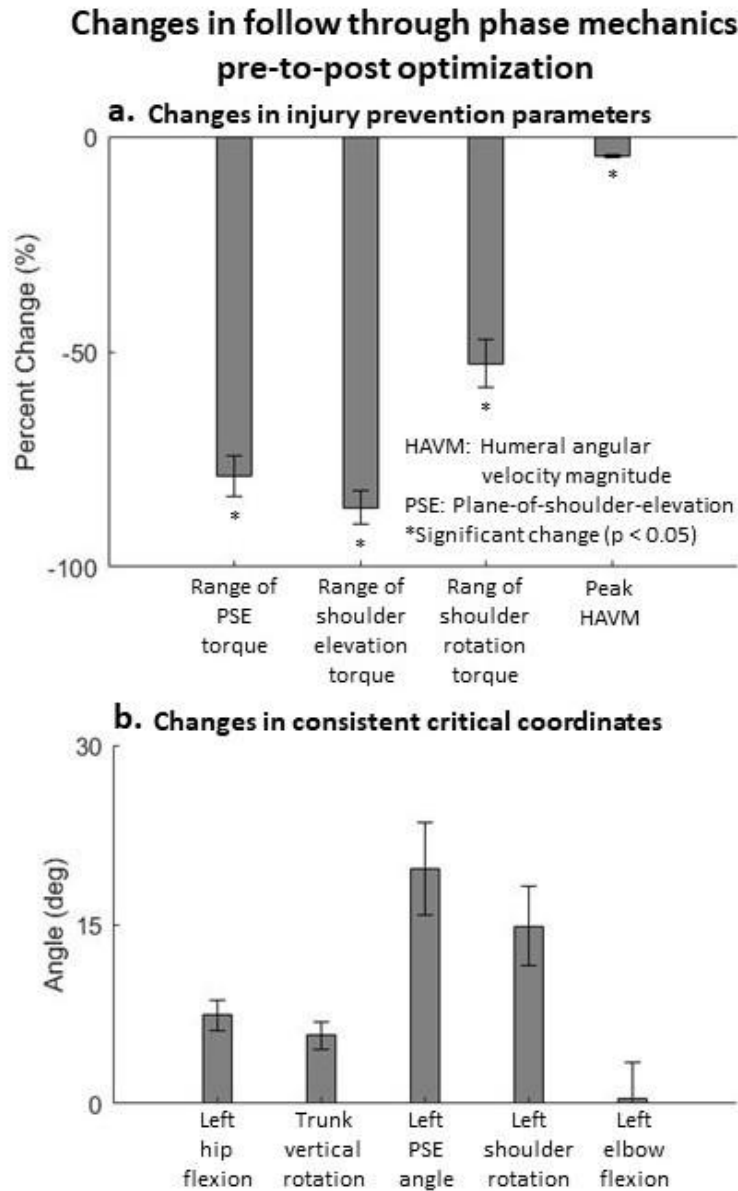


Figure 4.6. Changes in follow-through phase pre-to-post optimization. **4.6.a.** Change in injury prevention parameters. Mean $\pm$ standard error values across all participants are depicted. Note that in the statistical analyses, hierarchical linear modeling effectively compares trials of each participant pre-to-post optimization independent of other participants, rather than comparing all trials of all participants pre-to-post optimization. **4.6.b.** Coordinates that were consistently critical for at least 40% of the participants. These coordinates represent a general pattern that elicit the changes in the injury prevention parameters.

Change in consistent critical coordinates pre-to-post optimization for follow through phase

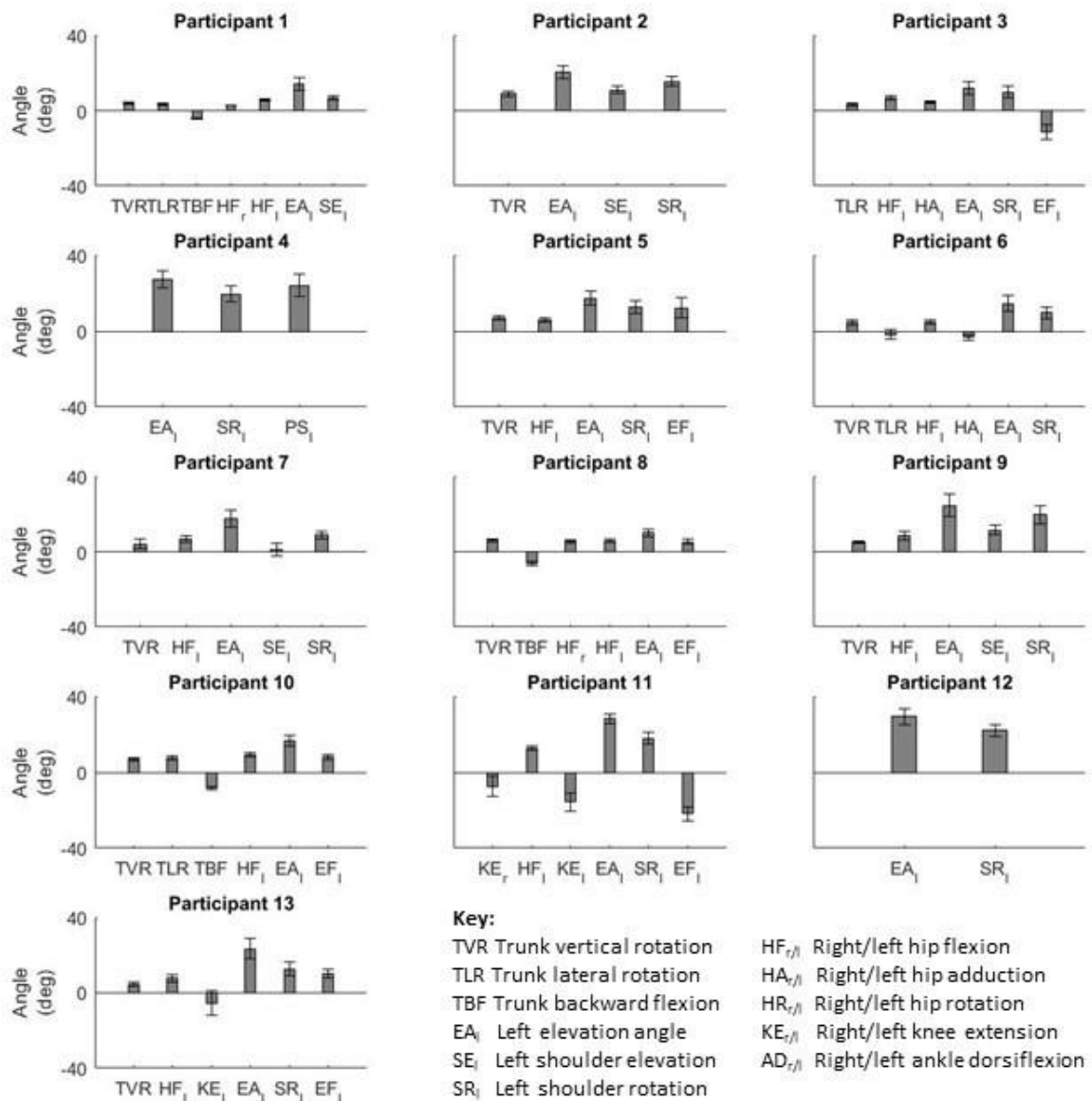


Figure 4.7. Consistent critical coordinates for all the participants during follow-through phase.

flexibility to focus on specific performance and injury prevention goals. It is not necessary that all athletes need to enhance performance and reduce the risk of injury at the same time. Certain athletes might only need to find ways to reduce their risk of injury, while others might want to only enhance certain performance parameters. Our goal-oriented approach to the optimization process is capable of accounting for these challenges. Since separate terms in the outer-level cost function account for different performance and injury prevention parameters, step functions can be used to address specific needs of each athlete. For example, if an athlete only wants to reduce the risk of injury, the performance parameters can be changed to step functions that contribute to the cost function only if the optimization reduces performance, similar to the cost function that does not allow peak HAVM to increase pre-to-post optimization. In this study, the goal-oriented cost function in the step 2 outer-level optimization of the follow-through phase ensures that the shoulder torques reduce by at least 10%. This value can be changed according to the needs of a given athlete, the goals of the coach, or for monitoring injury risk during rehabilitation. In this study, the percentage increase in peak height of the hitting wrist and the percentage increase in its forward velocity at peak height were weighted equally in the cost function (wrist term). We still recorded that the percent increase in forward velocity (25%) was much higher than the percent increase in peak height (1%). This is likely because anatomical constraints like arm length can only allow for a limited increase in the peak height. The forward velocity, on the other hand, which can be driven by the forward swing

of multiple lower body segments, has more freedom to increase. Note that maximum limits on torques were applied on all coordinates to avoid overload, but all these joints can work together synergistically to increase the forward velocity of the hitting wrist. From the point of view of specific needs of athletes and coaches, it is possible that an increase in only height or only forward velocity of the hitting wrist is required and not both at the same time. To account for this need, the wrist term can be broken down into separate terms, one each for height and forward velocity, and programmed such that the optimizer only increases one without decreasing the other. Additionally, separate optimizations for the power and follow-through phases also enable coaches to focus on specific phases of the movement, ones that they think are more important for a given athlete.

Our novel approach of tracking hypothetical performance trajectories was successful in finding kinematics with better performance parameters. During the power phase, the forward swing of the lower body is the primary mechanism to enhance performance without increasing the risk of shoulder injury (Supplementary Data 4.1). This entails increased hip flexion and increased knee extension of both legs pre-to-post optimization. Fig. 4.5 shows that hip flexion of the right and left legs were consistently critical for 91.7% and 41.7% of the participants, respectively, while knee extension of the right and left legs were consistently critical for 41.7% and 66.7% of the participants, respectively. At least one of these four coordinates was consistently critical for all participants, and at least three were consistently critical for 58.3% of the participants. These consistent

critical coordinates were determined based on their presence in at least 40% of trials of a participant and their presence in at least 40% of the participants. The number 40% was manually chosen as it helped us remove the critical coordinates that might be specific to certain trials or certain participants but keep enough trials or participants to find the generalized mechanism. The results of this study suggest that the forward swing of the lower body is the generalized mechanism driving the increase in the performance parameters without increasing the risk of shoulder injury. This is because the athletes are in the air and no external torque acts on them, conserving angular momentum. A forward swing of the hips needs to be balanced by a forward swing of the upper body, driving the hitting arm forward. The increased vertical rotation of the trunk pre-to-post optimization (consistently critical in 75% of the participants) aids this forward swing of the hitting right hand, increasing the forward velocity. The increased extension of the knees during the power phase would also drive the legs lower. Since the trajectory of center of mass of the body cannot be changed mid-flight, the lowering of the legs would drive the hitting hand higher. Similar results were also observed in a previous study (Gupta et al., 2015). Additionally, since the forward swing of the lower body drives the hitting arm, and not the shoulder, the torques at the shoulder do not increase, ensuring no additional risk of shoulder injury.

During the follow-through phase, trunk rotation with the hitting arm is the primary mechanism of reducing the risk of shoulder injury (Supplementary Data 4.2). This is accompanied by increased left hip flexion and increased left plane-of-

shoulder-elevation angle (bringing the left arm forward) pre-to-post optimization. Fig. 4.7 shows that at least one out of these three coordinates was consistently critical for all participants, at least two out of the three coordinates were consistent in 84.6% of the participants, and trunk vertical rotation was consistently critical in 69.2% of the participants. The follow-through phase entails stopping a fast-moving arm. Rotation of the trunk with the arm would transfer some of the load required to stop the arm from the shoulder to the bigger trunk segment, similar to stopping a whip. The trunk with its bigger muscles is better equipped to handle the load and save the smaller shoulder muscles that contract eccentrically to stop the fast-moving arm. As in the power phase, angular momentum must be conserved in the follow-through phase as well. This is achieved by an increased left hip flexion and increased left plane-of-shoulder-elevation angle pre-to-post optimization. The increase in the left hip flexion angle and the plane of left shoulder elevation angle is much higher than the vertical rotation of the trunk because the trunk is more massive and hence a greater displacement of the balancing segments is required to counter its angular momentum. It is also interesting to note that for certain trials, this mechanism of the trunk rotating with the hitting arm manifested itself in a different way. Supplementary data 4.3 shows the experimental and the optimal kinematics for the follow-through phase of a trial from participant 8. For this trial, the critical coordinates were all in the sagittal plane (trunk forward rotation, right hip flexion and right ankle dorsiflexion). Closer observation of this trial shows that the follow-through motion of the arm in the experimental motion was primarily in

the sagittal plane. Consequently, the trunk rotated in the same direction to unload the shoulder and the right hip flexion aided conservation of angular momentum. This suggests that the trunk vertical rotation was a consistent critical coordinate, while trunk forward flexion was only critical in a few trials because a majority of trials in this study featured the hitting arm moving diagonally across in front of the body during the data collection, while only a few trials featured the arm follow-through primarily in the sagittal plane during data collection. The trunk rotated with the direction of the arm follow-through to unload the shoulder in both cases.

Participant-specific optimization is important. Most of the trials followed the general mechanism described earlier to enhance performance parameters and reduce injury parameters. However, it is also important to note that 3.8% and 11.0% of trials during the power and follow-through phases, respectively, did not have even a single critical coordinate that matched the consistent critical coordinates that describe the mechanism we described above. This highlights the strength of our optimization technique. It is understandable that a small percentage of trials or participants would not follow the general pattern and our optimization technique is capable of accounting for these differences by optimizing each trial independently and tracking the experimental data ensuring that each trial of each participant can be optimized. A secondary advantage of this technique is that it can identify certain participants or participant's trials that deviate far from the general pattern and could potentially place the participant at a higher risk of injury.

As with most studies, ours met with limitations. First, the use of goal-oriented terms in the step 2 outer-level optimizations introduced step functions making the overall cost function discontinuous. This does not allow for gradient-based optimization algorithms that can handle a large number of design variables. This, however, did not impede the interpretation of results from our study, as the number of design variables in the step 2 outer-level optimization were only three and four in the power and follow-through phases, respectively. In a more complex study with a greater number of design variables, step functions might need to be replaced by continuous functions (Dembia et al., 2021; Serrancolí et al., 2019) to allow for gradient-based optimization. The second disadvantage of using goal-oriented terms in the outer-level cost functions is that some of these terms force the optimization to terminate once the goal is met, rather than at the global minimum. For example, the HAVM term only ensured that the peak HAVM did not increase but it did not encourage the outer-level optimization to decrease the peak HAVM pre-to-post optimization. This means that it is possible to have a movement pattern that is even better than the ones determined in this study. We acknowledge that this is a limitation, but it does not undermine the results of our study since we still succeeded in significantly enhancing performance parameters and significantly reducing injury risk parameters. On the other hand, goal-oriented optimization helps control the simulations and take specific needs of the athletes and coaches into account, an advantage that outweighs its limitations. The third limitation of our study is that we performed the outer-level optimization on the

power and follow-through phases separately. This introduces a discontinuity between the optimal posture at the end of power phase and posture at the start of the follow-through phase. It was necessary for us to perform the two optimizations separately since the goals of each optimization were different, and separate optimizations help with computational efficiency. Our results still determine both general and participant-specific mechanisms of increase in performance parameters and reduction in injury risk parameters, which are independent of starting posture. Additionally, different athletes and different trials of the same athlete had different starting postures, yet most of our trials still followed the general mechanism. Further research is needed to integrate the goals of different phases of movement into a single outer-level optimization, while keeping the optimization computationally reasonable. Fourth, we used ideal force/torque actuators to drive our models. This limits our ability to find specific muscles that drive the changes in performance and injury prevention parameters. The major reason for not including muscles in our model was that muscle models for trunk and shoulder capable of dealing with high velocity movement are still a work in progress. Our approach still allowed us to understand the mechanism that elicits the changes, and based on this information, experimental studies, better musculoskeletal models, or consultation with athletic trainers can identify specific muscles important to drive these changes. Fifth, the total number of accepted optimal simulations were different for power and follow-through phases. This was because more simulations violated the acceptance criteria of the power phase than

for the follow-through phase. This finding suggests that more research needs to be done to make the goal-oriented cost function terms and the regular cost function terms work together. Even though we rejected some optimal simulations, we were still able to generate a large number (313) of optimal whole-body, participant-specific simulations, increasing the external validity of our research.

Our research opens doors for a variety of future studies. Our computational framework can be used to find optimal movement patterns for other sports and musculoskeletal disorders. Simpler versions of this framework have been used for finding optimal movement patterns to reduce risk of ACL injury risk during unplanned side-stepping (Donnelly et al., 2012c) and single-leg jump-landing (Gupta et al., 2018b), but this is the first time that both performance and injury prevention aspects have been addressed in the same computational study of this kind. This is also the first time that goal-oriented cost functions have been used in computational biomechanics opening new ways to control simulations and address specific goals that sports coaches or doctors might want to achieve. From the point of view of this volleyball study, future research would entail validation of our findings in an experimental setting, identifying specific muscle groups that drive the consistent critical coordinates and ultimately change the performance and injury prevention parameters, and finding best ways to teach the optimal hitting patterns to athletes. Some techniques that could be employed to teach the optimal patterns are video-based implicit learning (Farrow and Abernethy, 2002; Williams et al., 2002), muscular training (Staynor et al., 2017; Weir, 2014; Weir et al., 2014),

real-time feedback-based learning (Barrios et al., 2010; Pizzolato et al., 2017), and large-scale interventions studies built on sound mechanics and behavior change principles (Donnelly et al., 2020).

4.6. Acknowledgement

We thank Jody Jensen for allowing us to use the data collected in her lab for this study.

CHAPTER FIVE

FROM THE FIRST FORM OF OPTIMAL DYNAMIC SIMULATION

GENERATION PROCESS TO THE SECOND: VALIDATION

5.1. Abstract

The first form of the optimal dynamic simulation generation (ODSG) process used so far in this work suffers from the significant limitation of computational time. It takes multiple days to find the optimal movement patterns, limiting the clinical relevance of these methods. Trajectory optimization is an alternate way of generating simulations that is more computationally efficient. Although the use of trajectory optimization to generate simulations has been validated, it has never been used to find optimal movement patterns (second form of the ODSG process), similar to the previous two chapters. In this validation work, we used two trials of two different participants from the landing data used in chapter 3. We applied the second form of the ODSG process to find optimal movement patterns that achieve the same biomechanical goals as required in chapter 3. We compared the optimal kinematics generated by the second form of the ODSG process and the ones generated in chapter 3. We then found that both methods were able to reduce the peak non-sagittal plane knee moments (vector sum of knee ab/ad-duction moment and knee internal/external rotation moment) by at least 40%. The optimal kinematics generated by both methods were almost identical, but the second form of the ODSG process required 50% less time. This validates the use of the second form of the ODSG process to find optimal movement patterns.

5.2. Introduction

Musculoskeletal modeling of the whole-body combined with simulation allows for “what if” questions to be asked, which are difficult, time intensive and

costly to be answered through a heuristic experimental approach (Delp et al., 2007; Dembia et al., 2021). Optimization methods with musculoskeletal modeling and computer simulations (the ODSG process) have been used to find optimal kinematics during high velocity sporting tasks to reduce the risk of injury (Donnelly et al., 2012c; Gupta et al., 2018a; Gupta et al., 2019b; Gupta et al., 2018b). These methods involve a two-step optimization process, where each step is an outer-level optimization (Reinbolt et al., 2011). Outer-level optimization consists of an optimization routine (outer-level) that controls in the simulation-generating (inner level) optimization process. The first outer-level is used to optimize the parameters of the simulation generating process to minimize the residuals in the simulation. Residuals represent dynamic inconsistency between the external and inertial forces. The second outer-level optimization is used to find the optimal movement patterns that address the biomechanical needs of the movement. This form of the ODSG process is very powerful but suffers from the limitation that it takes multiple days to find the optimal kinematics, restricting its clinical applicability.

In this study, we used a radically different approach to achieve the same objective of generating optimal kinematics to reduce the computational time of the ODSG process. This new form of the ODSG process involves a different way of generating simulations. The first form of the ODSG process uses the residual reduction algorithm (RRA) that performs an optimization at each time interval. In the second form, we used trajectory optimization to generate simulations. Trajectory optimization finds the states and controls of the simulation over the

entire simulation time period instead of performing optimization of the controls at each time frame like RRA does. The dynamic system is governed by continuous time dependent dynamics that are hard to solve as functions. To address this issue, trajectory optimization changes or “transcribes” the problem such that we solve for real numbers rather than functions (Betts, 2010). Direct collocation is a transcription method. It follows from single and multiple shooting algorithms. Single shooting essentially optimizes the values of the control trajectory based on boundary conditions (start and end of the control trajectory), making it slow and inefficient for complex problems. Multiple shooting divides the trajectory into multiple segments, called meshes, and applies the single shooting algorithm at each mesh, solving them in parallel, and applying continuity constraints at each mesh point. Direct collocation has proven to be even more efficient because of its formulation and implementation. Shooting methods explicitly calculate the derivatives and integrals of the trajectories to satisfy dynamic constraints. Implicit methods used in direct collocation, on the other hand, remove the need of numeric integration, making it computationally more efficient (Dembia et al., 2021; Falisse et al., 2019).

Direct collocation transcription helps solve for the trajectory of all simulation states and controls at the same time, rather than at each time point individually. The states of a simulation are the position and velocity at each degree of freedom (joint coordinate), and the controls are the amount of excitation representing the amount of use of the torque actuators across each joint coordinate. Direct

collocation uses an initial guess of the states and control trajectories. This guess is essentially the values of the states and controls at a finite number of points equally spaced across the time period of the simulation (mesh points), and the values in between the mesh points are filled with splines. At certain points of each mesh interval, called the collocation points, the spline slopes are matched to the values of the state derivatives computed based on dynamics. These values are computed using approximations based on the order of the splines being used (Betts, 2010). This removes the need for numerical integration. The number of collocation points depends on the order of splines that are fit between the mesh points. This leads to a problem with thousands of design variables, but since many of the design variables are independent of the others, the jacobian and hessian matrices are sparse (Topputo and Zhang, 2014), and gradient-based local optimization methods are able to generate the optimal solution.

Since trajectory optimization solves for values of all states and controls at all mesh points at the same time, in other words, solves for the complete simulation at once rather than one time point at a time, it makes this method of generating simulations much faster. A secondary advantage of using trajectory optimization is that it represents the human control system better. It is known that we react to upcoming events in our motion since we can sense that they are coming. For example, while landing, our lower leg muscles start to contract before we even touch the ground to prepare for impact. When generating simulations at each time point, the upcoming events are unable to influence the simulations. Consequently,

while generating forward dynamics simulation of landing, the muscles will not start to contract until the model actually touches the ground. Since muscles are subject to activation dynamics, that is, they take time to reach their peak or desired activation, this can lead to dynamic inconsistencies and give rise to residuals at the time of impact to account for the preparation for landing that was missing in the simulation. Since trajectory optimization solves for the entire trajectory of the states and controls at the same time, it allows the simulation to adjust to upcoming events and prepare accordingly. In other words, while generating simulations of landing, trajectory optimization will allow the simulation platform to know that the ground is coming and allow for appropriate preparation. Hence, trajectory optimization represents the human control system better and also removes the need for residuals in the simulations. This further reduces the computational complexity of the second form of the ODSG process, since we no longer need an equivalent of the first outer-level optimization whose objective is to reduce residuals. This makes this form of trajectory optimization based the ODSG process a single step process.

In musculoskeletal modeling, trajectory optimization using direct collocation transcription has been applied to generate simulations (Falisse et al., 2019), but since the implementation of direct collocation transcription is complex and requires arduous bookkeeping, this method of generating simulations never found widescale application. This issue was recently addressed: OpenSim Moco is a new software platform that allows users to use OpenSim models and generate simulations using trajectory optimization with direct collocation transcription

(Dembia et al., 2021). OpenSim Moco allows users to generate simulations using cost functions that represent the cost functions typically used by OpenSim simulation-generating algorithms like RRA, while the complex direct collocation transcription is taken care of at the software end.

Although the use of trajectory optimization to generate simulations has been validated, it has never been used to find optimal movement patterns (second form of the ODSG process), similar to the previous two chapters. The purpose of this validation work is to test the robustness of the second form of musculoskeletal modeling to find optimal kinematics. We used the two trials of two different participants from the landing data used in chapter 3. We used the second form of the ODSG process to find optimal movement patterns that achieve the same biomechanical goals as required in chapter 3. We compared the optimal kinematics generated by the second form of the ODSG process and the ones generated in chapter 3.

5.3. Methods

We used one trial each from two participants from the data of chapter 3. We used the same scaled, 37 degree of freedom model and inverse kinematics as used in chapter 3. The objective of the ODSG process is also the same: find the optimal movement pattern to reduce the peak of the vector sum of the knee ab/adduction moment and the knee int/ext rotation moment. The simulations were generated for the same time period as the one used in chapter 3. Since trajectory optimization can allow us to remove residuals from the simulations, the second

form of the ODSG process becomes a single step process. The cost function of the second form of the ODSG process was similar to that of the step 2 of the optimization process used in chapter 3. The cost function features reduced tracking of non-pelvis coordinates and increased the penalty for using the knee adduction and knee internal rotation actuators. The following overall cost function was used:

$$\min_{q, \dot{q}, x} \left[\int_{t_i}^{t_f} \left[\sum_{i=1}^6 w_p (q(t)_i^{exp} - q(t)_i^{sim})^2 + \sum_{i=1}^6 \frac{w_p}{5} (\dot{q}(t)_i^{exp} - \dot{q}(t)_i^{sim})^2 + \sum_{i=7}^{31} w_{np} (q(t)_i^{exp} - q(t)_i^{sim})^2 + \sum_{i=7}^{31} \frac{w_{np}}{5} (\dot{q}(t)_i^{exp} - \dot{q}(t)_i^{sim})^2 + \sum_{k=1}^{29} (x(t)_k)^2 + p \sum_{k=30}^{31} (x(t)_k)^2 \right] dt \right] \quad (5.1)$$

Where, $w_p = 1000$ was the weight of tracking the position of the pelvis coordinates, $w_{np} = 100$ was the weight of tracking the position of all non-pelvis coordinates, and $p = 10$ was the penalty of using knee adduction actuator and knee internal rotation actuators. The weights and factors were manually selected to best represent the same cost function as used in chapter 3. $q, \dot{q}$ and x are the values of the states, and the controls being optimized over the time period of the movement. The simulation is generated from the time t_i to t_f . The values of the states and the controls (excitations) are computed at each mesh point and splines filled between them. Twenty mesh points were spread across the weight acceptance phase, which typically only lasts about 70 ms. This results in a higher mesh density compared to what has been used in previous literature using direct collocation transcription to generate gait simulations (Dembia et al., 2021). A randomized initial guess of the states and the control trajectories was used.

We compared the difference in the lower limb and trunk kinematics of the optimal simulations generated in this validation work to the ones generated in chapter 3. Only the lower limb and trunk coordinates were compared since these were the ones that were critical in achieving the biomechanical goals in chapter 3.

5.4. Results

Table 5.1 displays differences in the kinematics and the peak non-sagittal plane knee moment (vector sum of knee ab/ad-duction moment and knee int/ext rotation moment) between the two optimal simulations. Fig. 5.1 demonstrates the mechanism of reducing the peak knee adduction moment for participant 2. Both optimal simulations followed the same pattern of reducing the lever arm of the ground reaction forces about the knee in the frontal plane to reduce the peak knee adduction moment. Generating optimal movement simulations of single-leg jump-landing in this study took less than six hours, while it took about 13 hours to achieve the same in chapter 3.

5.5. Discussion

This validation work found that both forms of the ODSG process were capable of finding optimal whole-body kinematics that reduce the peak non-sagittal plane knee loads during the weight acceptance phase of single-leg jump-landing by at least 40%, reducing the risk of ACL injury. The optimal kinematics patterns were almost identical, with the mean difference between the lower limb and trunk coordinates less than 1° , suggesting that they are nearly identical (Table 5.1). Both optimal simulations reduced the peak knee adduction moment in mechanically the

Table 5.1. Differences in key kinematics and kinetics of the optimal movement patterns generated by the two forms of the optimal dynamic simulation generation process for the two participants.

	Difference between optimal kinematics (lower body and trunk)	Reduction in peak non-sagittal plane knee moment using different forms of optimal dynamic simulation generation process	
		First form	Second form
Participant 1	0.81° (0.35°)	75%	63%
Participant 2	0.66° (0.32°)	45%	74%

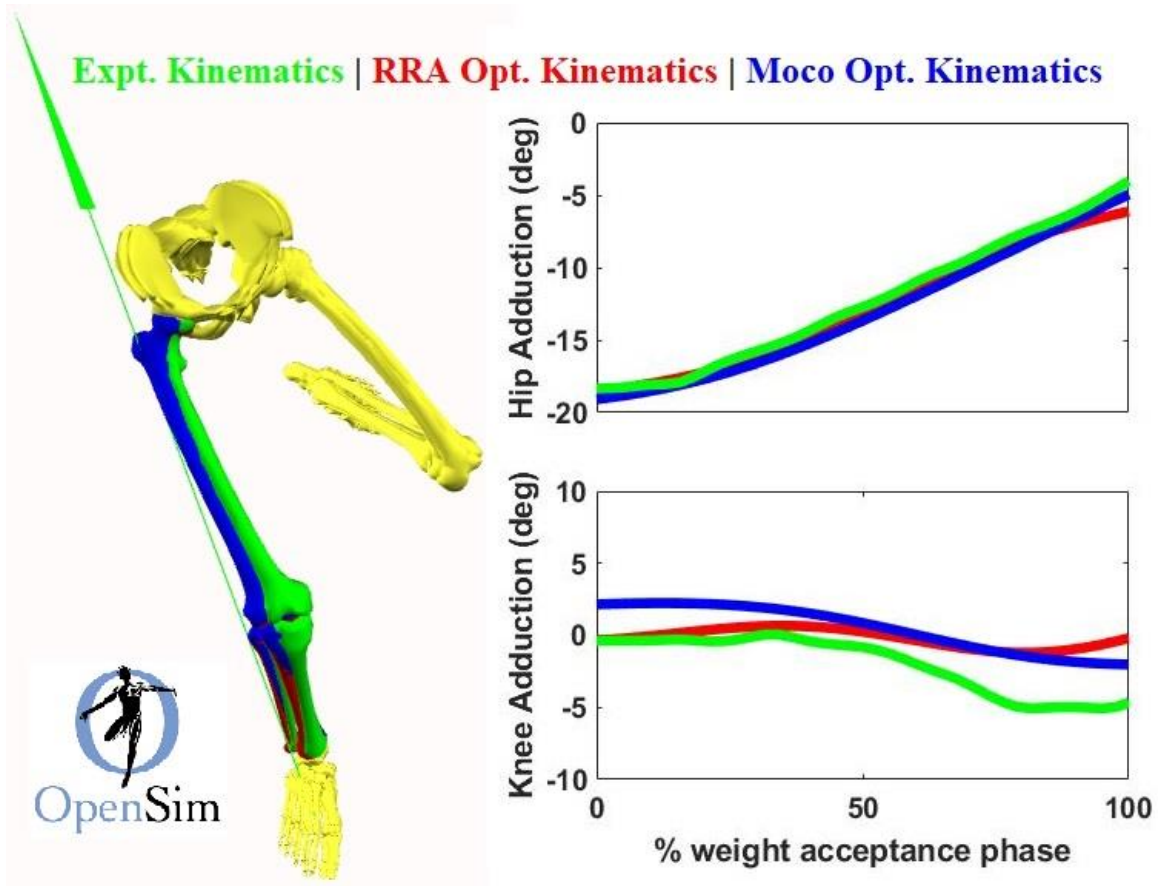


Figure 5.1. Visualization of mechanism of reduction of peak knee adduction moment during single-leg jump-landing for participant 2. Green represent experimental data. Red simulation is the optimal kinematics generated using RRA based first form of musculoskeletal modeling and blue simulation is the optimal kinematics generated using OpenSim Moco based second form of musculoskeletal modeling.

same way (Fig. 5.1), reducing the lever arm of the ground reaction force about the knee in the frontal plane. These results validate that the second form of the ODSG process generates reasonable optimal movement patterns to address biomechanical needs of a given movement.

The primary advantage of the second form of the ODSG process is that it took less than half the time to find the optimal kinematics compared to the first form. For slower clinical movements like gait, we expect that this time to be even less, making the ODSG process a clinically relevant tool. For example, a patient could be tested in a motion capture lab in the morning, and the clinician could be presented with the optimal movement pattern in the afternoon.

5.6. Acknowledgement

We thank Caroline Finch, David Lloyd and Bruce Elliott for providing experimental data (NHMRC grant: 400937).

CHAPTER SIX

STUDY IV: OPTIMAL GAIT PATTERNS THAT REDUCE PEAK KNEE ADDUCTION MOMENT WITHOUT INCREASING PEAK KNEE FLEXION/EXTENSION MOMENT: IMPLICATIONS FOR PROGRESSION OF KNEE OSTEOARTHRITIS

6.1. Abstract

Force between the medial femoral condyle and the tibial plateau is the primary cause of medial compartment knee osteoarthritis (OA). High medial contact force (MCF) during gait has been shown to be correlated to both knee adduction moment (KAM) and knee flexion/extension moment (KFM). In this study, we used an efficient form of the optimal dynamic simulation generation (ODSG) process to find optimal gait kinematics that reduce the peaks of the KAM, without increasing the peaks of the KFM. This can potentially reduce the MCF and hence the progression of knee OA. We used gait data from four knee OA participants. Our simulations decreased both peaks of the KAM by at least 80% without increasing either peak of the KFM. We found that the primary mechanism followed by simulations of all participants was to increase the step width. This leads to a reduction of the lever arm of the ground reaction force vector about the knee in the frontal plane, in turn reducing the KAM. Interestingly, all four participants followed different patterns of kinematic changes to achieve this decrease in lever arm, featuring different combinations of increase in knee abduction, increase in hip abduction and increase in foot progression angle. Differences in changes in kinematic patterns to achieve the biomechanical goals of the movement demonstrate the importance of participant-specific modeling. The most significant achievement of this study is that our computationally efficient methods were able to find the optimal gait patterns within 15 minutes compared to multiple days that

the previous iterations of these methods took, making our process of finding optimal movement patterns clinically relevant.

6.2. Introduction

Knee osteoarthritis (OA) affects 12.1% of all adults above the age of 60 years in United States (Lawrence et al., 2008) and costs \$140,300 per patient over their lifetime (Losina et al., 2015). Knee OA is a degenerative disease where repeated transmission of force between the weight-bearing femoral condyle with the tibial plateau causes degeneration of the bone tissue. Degenerative in nature, it primarily affects the older population. Knee OA causes stiffness, swelling, and pain in the knee, which increases with more vigorous movements (Lespasio et al., 2017). This limits the physical wellbeing of the patient and leads to higher social and economic cost. Knee OA has been attributed to a number of causes ranging from biomechanical pattern of movement, age, gender, hormones, race, genetics, diet, obesity, previous injury at the knee, physical activity, alignment of the knee, and laxity in the knee (Heidari, 2011; Zhang and Jordan, 2010).

Among activities of daily living, the stance phase of gait transmits the maximum amount of force through the knee (Trepczynski et al., 2014). This is primarily because in most of the other activities of daily living, both the legs support the body weight while in the stance phase of gait, only one leg supports the body weight. Additionally, the contact between the medial femoral condyle and the tibial plateau generally carries the majority of body weight during gait (Winby et al., 2009; Zhao et al., 2007). Because of this reason, knee OA is more prevalent in the

medial compartment of the knee. Hence, the study of knee OA has typically been focused on medial knee contact force during the stance phase of gait (Fregly et al., 2012). The exact measurement of the medial contact force (MCF) is difficult without placing a sensor at the contact surface. It has been observed that both the MCF and the knee adduction moment (KAM) follow similar curves with two peaks, one in the early stance and one in late stance. KAM has also been found to be highly correlated to MCF, and higher KAM has been recorded in knee OA patients (Manal et al., 2015; Ogaya et al., 2014). Therefore, KAM has traditionally been used as a surrogate measure for MCF, to study knee OA biomechanically (Baliunas et al., 2002).

As a relief mechanism, patients with knee OA have been observed to make modifications to their gait like trunk lean. In addition, researchers have also studied the effects of a variety of gait modifications on the KAM such as changing gait speed, step width, toe progression angle, and medial thrust. The general mechanism is to reduce the lever arm of the ground reaction force (GRF) about the knee, which reduces the KAM. Trunk lean moves the center of mass (COM) over the knee, while most of the other gait modifications bring the knee closer to the GRF vector. These gait modifications reduce the lever arm of the GRF vector about knee. The natural gait modification of trunk lean has been the most effective, but it is not popular among the patients as it forces them to change their gait and looks considerably awkward. All the gait modifications proposed by researchers have had mixed effects on the KAM. Gait modifications like toe-out and increased

speed only reduce the second peak (Guo et al., 2007; Landry et al., 2007) while toe-in and reduced gait speed only reduce the first peak (Lynn et al., 2008; Robbins and Maly, 2009) with a few exceptions. Increasing step width has been shown to reduce the KAM as well (Fregly et al., 2008) but the most effective gait modification that reduces both the peaks of KAM by as much as 30%, without considerably changing the gait pattern has been medial thrust (Fregly et al., 2007). Fregly et al. (2007) used the ODSG process to predict a gait pattern that would reduce the KAM. The simulations found that if one brings the knee more medial while walking, both KAM peaks reduce. Follow-up studies validated this finding (Schache et al., 2008). Medial thrust, however, failed as a preventive solution to knee OA because it failed to greatly reduce the MCF, especially its first peak (Walter et al., 2010).

The reason why gait modifications have typically failed to reduce the MCF has been attributed to the finding that the MCF is correlated to both knee adduction moment and knee flexion-extension moment (KFM) (Manal et al., 2015; Ogaya et al., 2014; Walter et al., 2010). Gait modifications typically reduce the KAM but increase the KFM and hence fail to reduce the MCF (Walter et al., 2010). Hence, it is essential to find gait modifications that reduce peak KAM without increasing peak KFM during gait (Ulrich et al., 2020). A recent experimental study tested if gait modifications can reduce peak KAM without increasing peak KFM during gait (Ulrich et al., 2020). It concluded that gait modifications can achieve a decrease in peak KAM without increasing peak KFM, but failed to identify ways to find participant-specific gait modifications.

In this study, we used the second form of musculoskeletal modeling validated in chapter 5 to find optimal participant-specific gait patterns (Gupta et al., 2020) that reduce both peaks of the KAM without increasing either peak of the KFM. We used trajectory optimization in OpenSim Moco, combined with appropriate cost functions capable of generating optimal kinematics based on previous chapters, to generate simulations at a higher computational efficiency.

6.3. Methods

6.3.1. Participants and experimental data collection

We used data from a pool of gait data that was collected for a separate study (Edmonds et al., 2016). The 15 participants of this study (10 men, 5 women) were above the age of 60 years, clinically diagnosed with knee OA, and had no prior surgery besides arthroscopy. Participants wore the UWA marker set (Besier et al., 2003; Donnelly et al., 2012b). Marker movement data was collected using a 11 camera (7 MX cameras and 4 T40 cameras) Vicon motion capture system (VICON MX, Oxford Metrics Limited, Oxford, UK) at 100 Hz. At the same time, ground reaction forces were collected from two AMTI force plates (MCA-6, Advanced Mechanics Technology Incorporated, Watertown, USA) at 2000 Hz. The movement and force plate data were synchronized in the Vicon Giganet control box and within the Vicon Nexus software (Vicon Peak, Oxford Metrics Ltd., UK). This data was collected at the Gait Laboratory at the School of Sports Science, Exercise, and Health at The University of Western Australia and ethical approval for the data collection was obtained by the Human Research Ethics Committee of

The University of Western Australia. Written informed consent was obtained from each participant before data collection.

Data collection involved participants walking back and forth in a straight line in the motion capture lab. Only the trials where each foot was completely within the boundary of one force plate and the other foot within the boundary of the other force plate were analyzed. This is necessary to ensure that each force plate collects the data from only one foot, and this data can be applied as external forces to the respective foot during the musculoskeletal modeling process. Since the force plates were adjacent to each other, each of the qualified trials had the data of consecutive heel strikes (one from each leg). The study for which the data was collected was aimed at assessing the effect of knee taping on pain, spatiotemporal parameters, knee kinetics, and knee kinematics. Gait data was collected under three different conditions: 1) no taping, 2) sham taping where tape was loosely attached, and 3) therapeutic taping where taping was applied to alleviate pressure from the infra-patella fat pad (Edmonds et al., 2016). At least six trials that qualified with the desired foot placement on the force plates were collected in each condition, and the order of the conditions was randomized. It was found that therapeutic taping reduced the self-reported pain but no difference in the spatiotemporal, knee kinetics or knee kinematics variables was observed between the three taping conditions (Edmonds et al., 2016). For this reason, we treated all gait trials from the dataset equally without any bias to the taping condition under which the trial was collected. Unfortunately, since Edmonds et al. (2016) only

aimed to study the effect of taping on the knee, they only used a lower limb marker set on most of the participants. For our study, we needed the trunk motion since changes to the trunk motion can influence the KAM (Hunt et al., 2008). Hence, for this study we used only the four participants from the dataset that wore the trunk markers (three men, one woman).

6.3.2. Musculoskeletal model and foot contact model

For musculoskeletal modeling, we used the generic gait 2392 model freely available in OpenSim (simtk.org). This model has 23 degrees of freedom (three at the hip, one at the knee and three at the foot for each leg, three at the trunk, and six at the pelvis root segment with respect to the ground). We added the abduction/adduction and internal/external rotation degrees of freedom to the knees to allow for study that involves KAM. In this study, we used Hunt-Crossley spheres as foot contact model (Falisse et al., 2019; Sherman et al., 2011). Hunt-Crossley spheres are spheres added to the base of the foot that act as elastic elements. The more they penetrate the ground, the higher the GRF. These spheres are also accompanied by a friction model that applies a frictional force in the direction opposite to the relative direction of motion between the ground and the sphere in the horizontal plane (Sherman et al., 2011). Multiple spheres are generally added across different areas of the foot to generate a total GRF that accounts for the effect of movement of different parts of the foot on the total GRF. Falisse et al. (2019) optimized the parameters of a foot contact model using six Hunt-Crossley spheres spread across the foot for a single healthy participant. Falisse et al. (2019)

also found that that using the foot contact model with optimized parameters of the Hunt-Crossley spheres produced the same total GRF compared to the foot contact model without optimized parameters, with almost identical kinematics. The primary reason is that that these spheres are very stiff, and even minor changes in foot movement can produce a large change in the GRF. Therefore, minimal changes in kinematics can produce enough changes in GRF such that the parameters of the foot contact model do not influence the simulation. For this reason, we used the foot contact model with the optimal Hunt-Crossley spheres parameters generated by Falisse & colleagues (Falisse et al., 2019), scaled to each participant of our study. We used the model with optimal Hunt-Crossley spheres parameters as opposed to the generic foot contact model simply because they were optimized to human anatomy. Since this model locked the metatarsophalangeal (mtp) joint of the foot, we did too. The same foot contact model has been used for all participants of another study. This study also found good correlation between the GRF generated by the foot contact model and the experimental GRF (Lin and Pandy, 2017).

Use of a real foot contact model as opposed to ZMP computations as used in chapter 3 allows for more accurate foot-ground contact modeling. This is because the ZMP computations act as a check to ensure that the center of pressure (COP) of a new movement is below the base of support (the foot). They do not actively produce the GRF based on the motion of the foot. A foot contact model, on the other hand, calculates the GRF based on the interaction of the foot

with the ground, which is a more accurate representation of human movement. Another advantage of using a foot contact model over ZMP computations is that during the double stance phases, the base of support is very large, spanning across both feet. Hence, the ability of ZMP computations to ensure dynamic consistency is limited in this scenario. Chapter 3 dealt with single-leg jump-landing and hence the base of support was only one foot, making ZMP computation enough to ensure dynamic consistency, but the study of gait in this study, which involves double support phases, calls for a real foot contact model.

We scaled the generic model and the foot contact model with optimal Hunt-Crossley spheres parameters to each participant using a static trial. This was followed by inverse kinematics to find the body coordinates of the gait trials. We then performed inverse dynamics to find the KAM and KFM before the optimization step. The inverse kinematics and inverse dynamics were only performed from 50 ms before the heel strike until 40 ms after toe-off of the foot of the leg with knee osteoarthritis. This is because the progression of knee OA is associated with the knee loads during the stance phase since the leg carries the entire body weight (Fregly et al., 2012). Scaling and inverse kinematics were performed in OpenSim v4.1 (simtk.org). Inverse kinematics only generates the position of each body coordinate. The states reporter tool in OpenSim v4.1 was used to generate states (position and velocity of each body coordinate) corresponding to the inverse kinematics generated movement. For each participant, we chose five trials that recorded the highest KAM values and used these trials for further analyses.

6.3.3. Optimal dynamic simulation generation

In this study, we used trajectory optimization to generate simulations. In addition, we used our knowledge of designing cost functions from the previous chapters to perform the ODSG process to find optimal gait patterns that would potentially reduce the progression of knee OA by reducing peak KAM, without increasing the KFM. To do so, we used ideal force/torque actuators to drive our model. The maximum force capacity of each of these actuators was the same as the generic RRA parameters of the gait 2392 model.

To ensure that the optimization platform is able to generate new simulations, we tracked the original kinematics such that the pelvis coordinates were tracked with a high weight (1000) to ensure the forward motion of the simulation, the trunk and the non-affected leg were tracked with a lower weight (500), and the coordinates of the affected leg were tracked with the least weight (100). The coordinates of the trunk and the non-affected leg were tracked higher than those of the affected leg to avoid excessive change in trunk lean, which is typically accompanied by a counter balancing increase in hip abduction of the non-affected leg. Velocity of each coordinate was tracked with one-fifth weight of the position value of that coordinate (Delp et al., 2007). States tracking was the first cost function. Our models had 50 states, position and velocity of the 25 coordinates (three for the hip, three for the knee, one for the ankle, one for the subtalar joint for each leg, three for the trunk and six for the pelvis).

The sum of squared excitation of all the actuators was the other cost function. Since we wanted to reduce the KAM and not increase the KFM, the excitation of the knee adduction actuator and knee flexion actuator was weighted more than the excitation of other actuators by a factor. Our model had 19 torque actuators, one for each coordinate except the pelvis coordinates. Actuators at pelvis coordinates represent the residuals, and since trajectory optimization is capable of working without residuals, we did not include them in our simulations.

Overall cost function:

$$\min_{q, \dot{q}, x} \left[\int_{t_i}^{t_f} \left[\begin{aligned} &\sum_{i=1}^6 w_p (q(t)_i^{exp} - q(t)_i^{sim})^2 + \sum_{i=1}^6 \frac{w_p}{5} (\dot{q}(t)_i^{exp} - \dot{q}(t)_i^{sim})^2 \\ &+ \sum_{i=7}^{17} w_t (q(t)_i^{exp} - q(t)_i^{sim})^2 + \sum_{i=7}^{17} \frac{w_t}{5} (\dot{q}(t)_i^{exp} - \dot{q}(t)_i^{sim})^2 \\ &+ \sum_{i=18}^{25} w_{OA} (q(t)_i^{exp} - q_i^{sim})^2 + \sum_{i=18}^{25} \frac{w_{OA}}{5} (\dot{q}(t)_i^{exp} - \dot{q}_i^{sim})^2 \\ &+ w_e \sum_{k=1}^{17} (x(t)_k)^2 + w_e f_{add} (x(t)_{add})^2 + w_e f_{fe} (x(t)_{fe})^2 \end{aligned} \right] dt \right] \quad (6.1)$$

Where, $w_p = 1000$ was the weight of tracking the position of the pelvis coordinates, $w_t = 500$ was the weight of tracking the position of the trunk and non-affected leg's coordinates, $w_{OA} = 100$ was the weight of tracking the position of the affected leg's coordinates, $w_e = 10$ was the weight on excitation of all the actuators, $f_{add} = 100$ was the factor by which the weight on excitation of the knee adduction actuator ($x(t)_{add}$) was increased, and $f_{fe} = \left(\frac{100 \text{ Nm}}{\text{peak KFM (in Nm)}} \right)^2$ was the factor by which the weight on excitation of the knee flexion-extension actuator ($x(t)_{fe}$) was increased. The weights and factors were manually selected. The values of states and controls (excitations) are computed at each mesh point and splines filled between them. The initial time t_i was 50 ms before the heel strike and

final time t_f was 40 ms after the toe-off. There was one mesh point every 10 ms. This results in a higher mesh density compared to what has been used in previous literature using direct collocation transcription to generate gait simulations (Dembia et al., 2021), implying more accurate results.

We wanted to find optimal gait patterns that are not too different from the collected data so that these gait modifications can be easily learned. For this reason, we used the original motion states as the initial guess for the model states, rather than a random initial guess as used in chapter 5. The initial guess of the excitations of the actuators, except for the knee adduction actuator, were the trajectories of the inverse dynamics torque across each coordinate divided by the maximum torque capacity of the actuator across that coordinate. The initial guess for the excitations of the knee adduction was a trajectory of zeros. In a way, our initial guess represents the ideal solution and asks the optimization process to solve for dynamic constraints and generate a simulation close to the initial guess. Time taken for each optimization to converge was recorded.

6.3.4. Post-hoc analyses

Since there were only four participants in this study, we did not run statistics. This is because the low number of participants restrict external validity of our results, potentially causing type 1 error. We instead took advantage of the low number of participants to study each one individually. For each participant, we studied the change in both peaks of the KAM and the KFM pre-to-post optimization.

To find the key kinematics change that elicits the change in peak KAM and KFM, we computed the critical coordinates for each trial, similar to a previous study (Donnelly et al., 2012c). Critical coordinates are the coordinates whose absolute value of average change pre-to-post optimization is greater than the absolute value of average value plus one standard deviation of changes in all coordinates pre-to-post optimization. To find a general pattern of key kinematic changes for each participant, we also computed the consistent critical coordinates. The consistent critical coordinates are the coordinates that were critical for at least four out of the five trials of the participant. We also computed the change in step length, step width, step time and foot progression angle heel strike of the affected leg, pre-to-post optimization. The step length, step width and step time were measured based on the position of the ankle joint centers, measured between heel strike of the affected leg and heel strike of the non-affected leg.

To understand the mechanism of change in peak KAM, we also computed the change in lever arm of the net GRF about the knee in the frontal and sagittal planes (averaged over the stance phase of the affected leg). The lever arm of the GRF influences the KAM, and studying the lever arms can help us understand the mechanism of the change in KAM (Hunt et al., 2008).

Additionally, we recorded the time taken to perform the ODSG process to assess the computational cost.

6.4. Results

For each participant, both peaks of the KAM reduced, without increasing either peak of the KFM (Fig. 6.1). Consistent critical coordinates for all participants are shown in Fig. 6.2. To better understand the effects of the key kinematic changes, changes in step length, step width and step time are shown in Fig. 6.3. Fig. 6.4. shows the changes in foot progression angle of the affected leg at the heel strike. Fig. 6.3 suggests that all participants followed a strategy of increasing the step width, and Fig. 6.4 suggests that all participants, especially participant 2, also increased the foot progression angle of the affected leg at the heel strike. Supplementary data 6.1 and 6.2 show the frontal and sagittal plane views of the kinematics of both pre- and post-optimization during stance phase of the affected leg from one trial from each of the four participants. The net effect of all these kinematic changes was that the lever arm of the GRF about the knee joint center of the affected leg decreased, in turn reducing the KAM (Fig. 6.5). Fig. 6.6 shows the time taken to find the optimal kinematics.

6.5. Discussion

In this study, we used the ODSG process to find optimal gait patterns that could reduce the progression of knee OA by reducing the peaks of the KAM without increasing the peaks of the KFM (Manal et al., 2015; Ogaya et al., 2014; Walter et al., 2010). We were able to reduce both peaks of KAM for all the participants by at least 80% without increasing either peak of the KFM (Fig. 6.1). We found that the common distinguishing feature that drove this change in the KAM was the increase

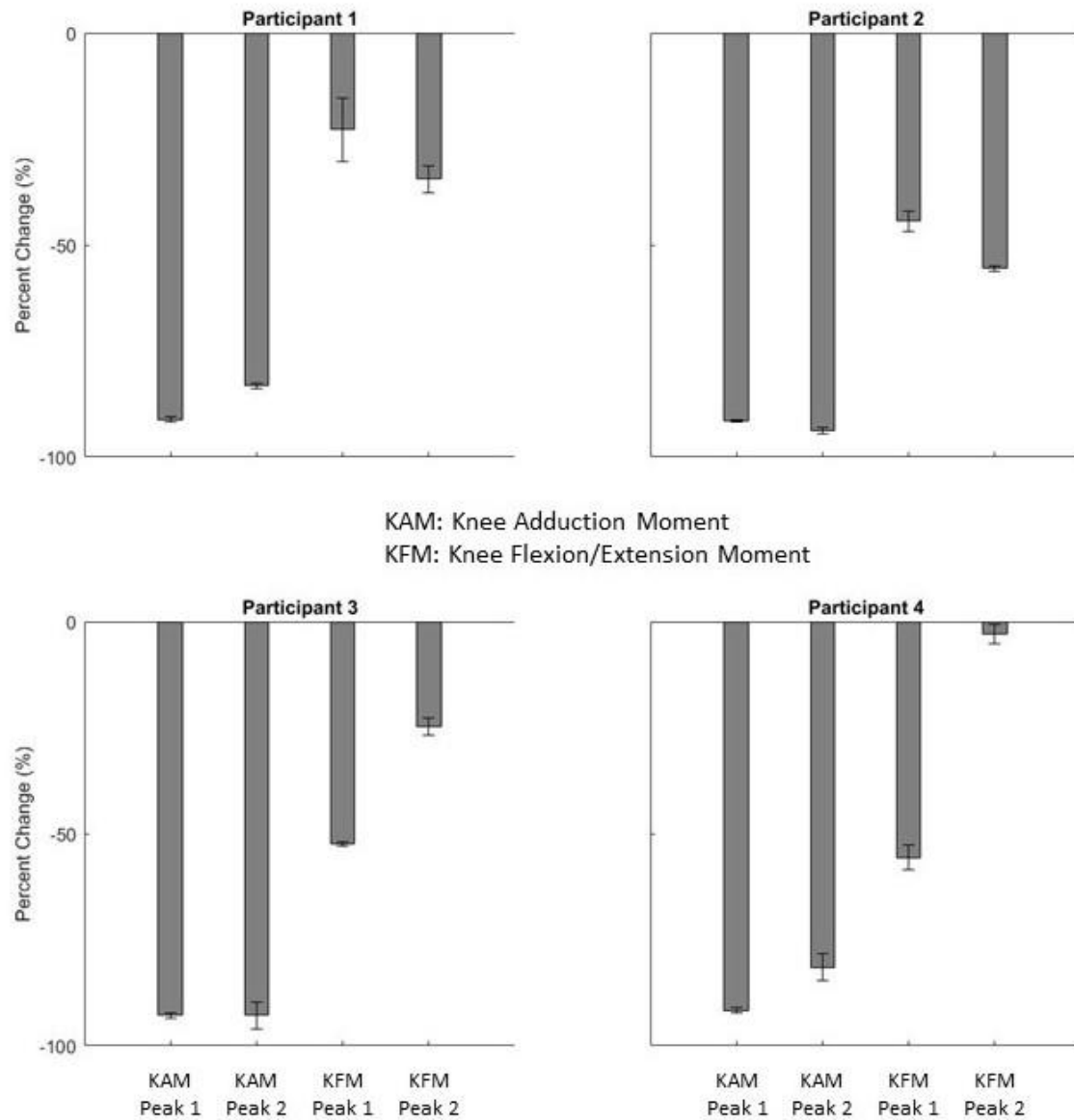


Figure 6.1. Percent changes (mean $\pm$ standard error), pre-to-post optimization for each participant, in peaks of knee adduction moment and knee flexion/extension moments.

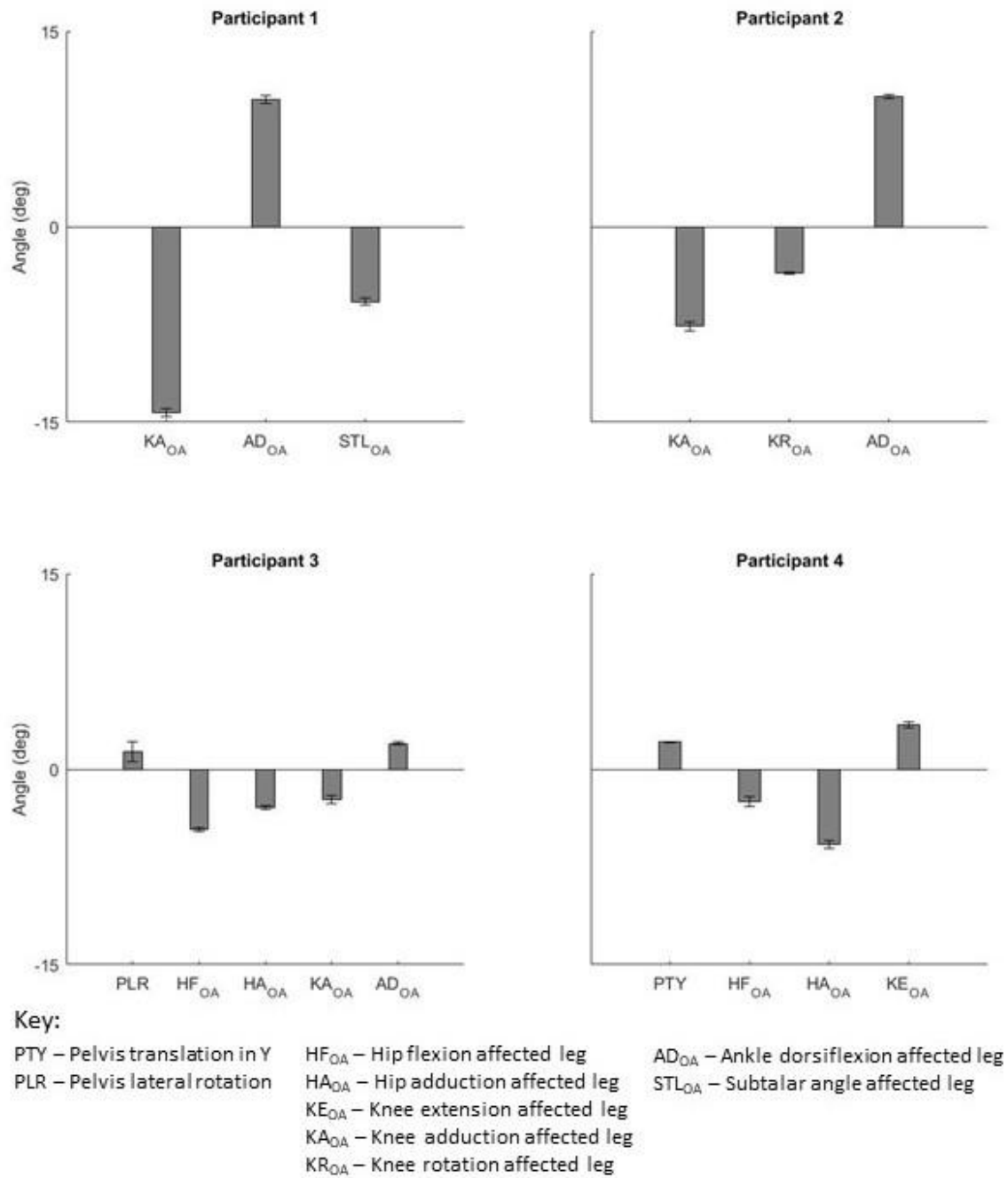


Figure 6.2. Consistent critical coordinates for each participant and the changes (mean $\pm$ standard error) in consistent critical coordinates.

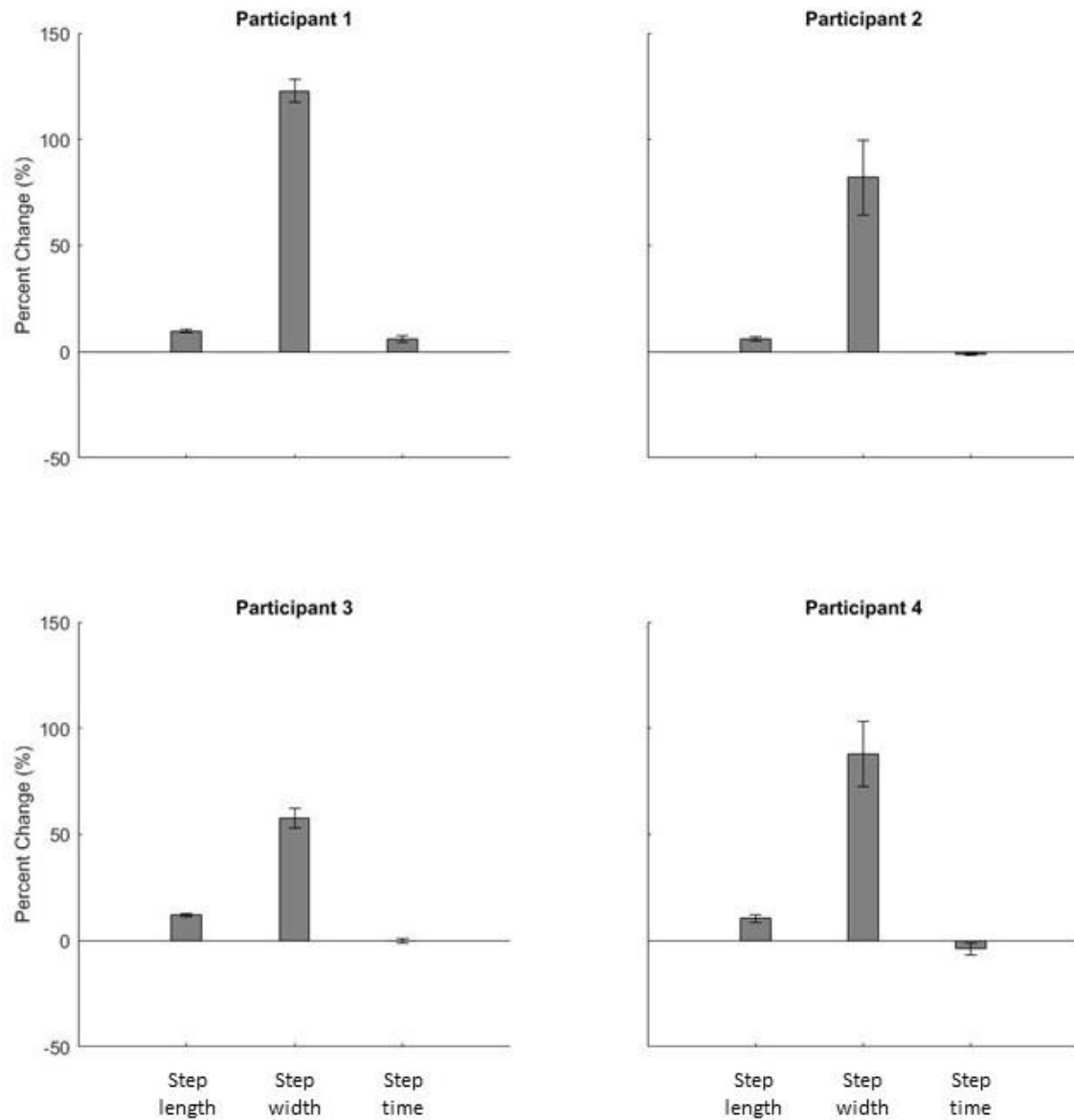


Figure 6.3. Percent changes (mean $\pm$ standard error), pre-to-post optimization for each participant, in key gait parameters measured based on the ankle joint center positions at heel strike of the affected and non-affected leg.

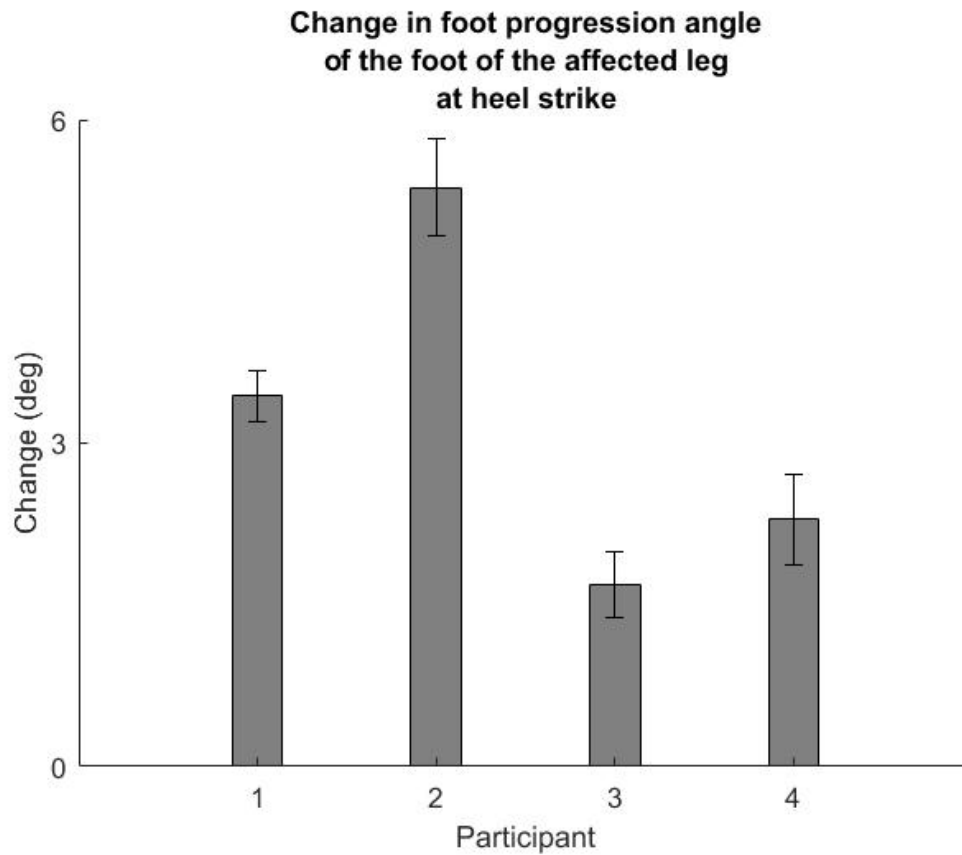


Figure 6.4. Change (mean $\pm$ standard error), pre-to-post optimization for each participant, in foot progression angle of the affected leg at heel strike.

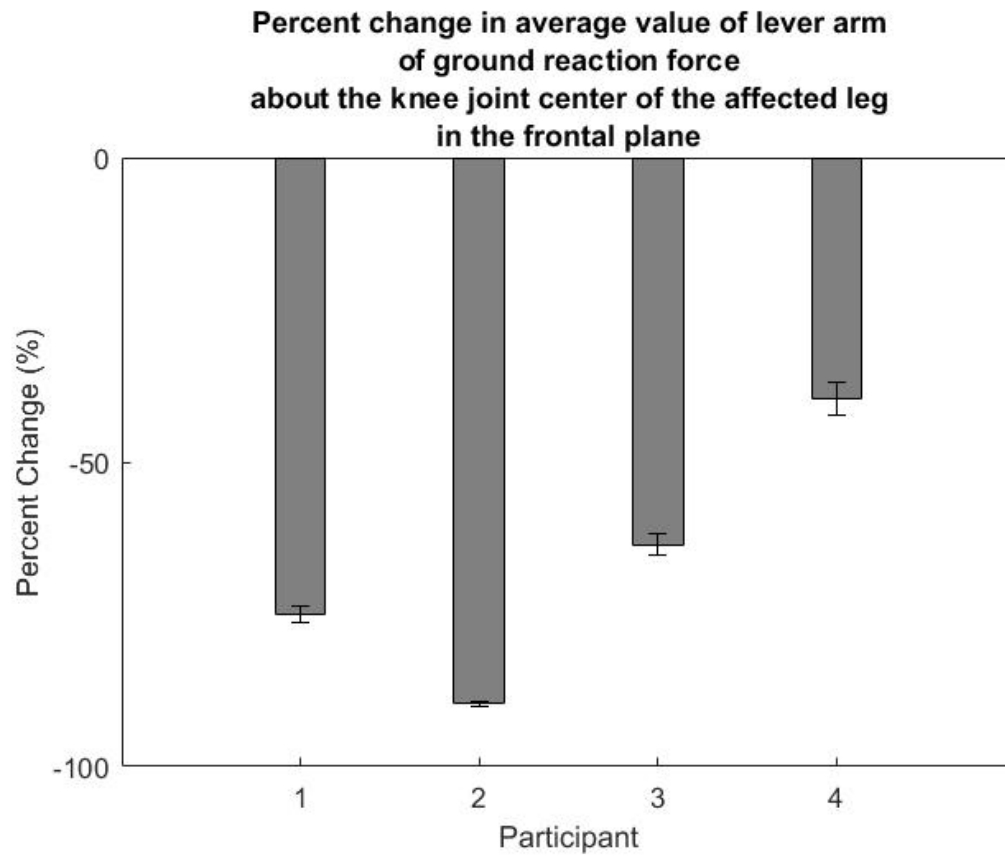


Figure 6.5. Percent change (mean $\pm$ standard error), pre-to-post optimization for each participant, in the average value of lever arm of ground reaction force about the knee joint center of the affected leg in the frontal plane.

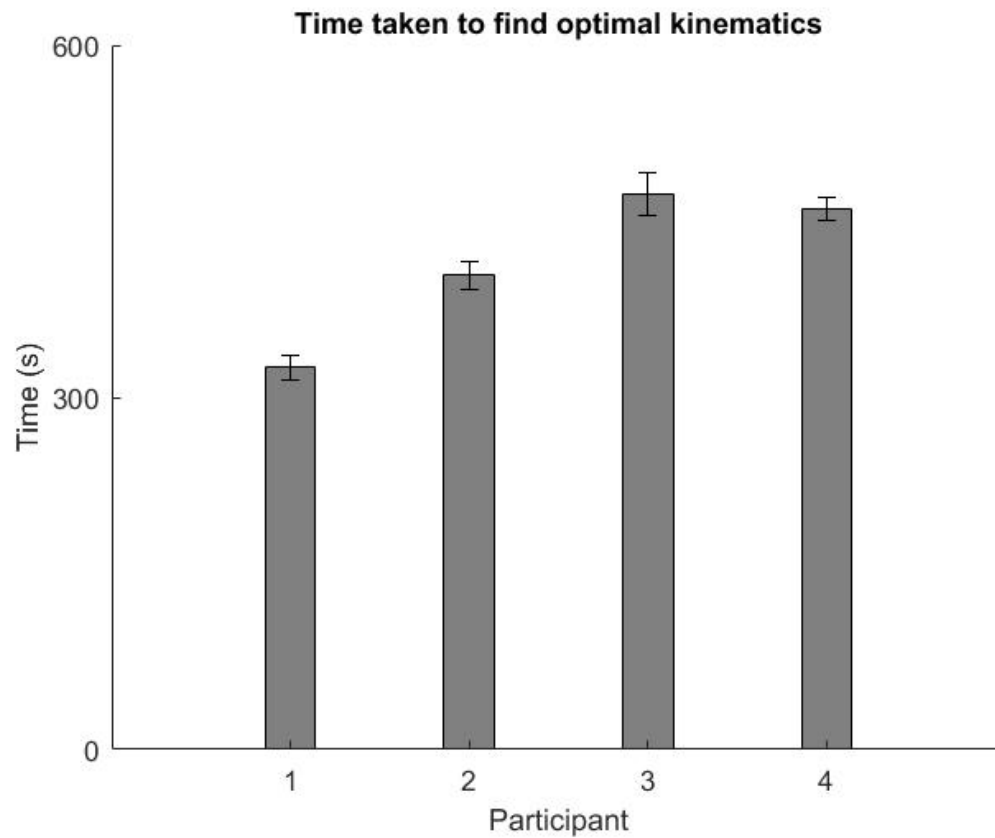


Figure 6.6. Time taken (mean $\pm$ standard error), for each participant, to find optimal gait patterns.

in step width. All participants increased their step width by at least 50% (Fig. 6.3). Increase in step width reduced the moment arm of the GRF about the knee joint center in the frontal plane, reducing the KAM. All participants recorded at least 30% reduction in the average value of lever arm of the GRF across the knee joint center in the frontal plane (Fig. 6.5). This mechanism of reduction of the KAM by an increase in step width is consistent with previous literature (Fregly, 2008). From the standpoint of mechanics, this effect is similar to the medial thrust gait (Fregly et al., 2007). In medial thrust, the knee is brought more medial compared to the foot to reduce the lever arm of the GRF about the knee joint center in the frontal plane. Increasing the step width essentially achieves the same objective by placing the foot more lateral compared to the knee.

Interestingly, we found that even though each participant reduced the peaks of the KAM by increasing the step width, they followed different mechanisms to do so (Supplementary data 6.1). Participant 1 and 2 achieved this by primarily increasing the knee abduction of the affected leg (Fig. 6.2). Participant 3 increased abduction of both the hip and knee of the affected leg (Fig. 6.2). Participant 4 primarily increased the hip abduction (Fig. 6.2). In addition, participant 2 also increased the foot progression angle by increasing the knee external rotation (Fig 6.2 and 6.4). An increase in foot progression angle has also been suggested in the literature as a mechanism by which the lever arm of the GRF about the knee joint center in the frontal plane can be reduced (Guo et al., 2007). The fact that we observed a different pattern of kinematic changes for each of the participants is

consistent with the findings of a recent experimental study that tested if gait modifications can reduce peak KAM without increasing peak KFM during gait (Ulrich et al., 2020). This experimental study, however, tested a predefined combinations of gait modification lacking participant specificity. The fact that we observed a different pattern of kinematic changes for each participant is a significant find. To some extent, it explains why no single gait modification proposed in the literature has been truly successful. Our results suggest that participant-specific optimization of movement is essential. Other studies have also found that patient specificity is important to improve efficacy of gait modifications (Uhlrich et al., 2020). While multiple gait modifications like medial thrust, increased step width, or increased foot progression angle may help, the degree to which each is employed is participant-specific. This finding of diversity in kinematic patterns is also important from a clinical perspective as it implies that participant-specific care is a key element to preventive care.

The most significant achievement of this study is its computational efficiency. This study can potentially change how we perform experimental science. Although a powerful tool, the ODSG process has not found common use because of its computational complexity. The first form of the ODSG process takes multiple days to find the optimal movement pattern. The large amount of time taken to find the solution puts the first form of the ODSG process outside of the time frame of clinical relevance. With the use of trajectory optimization in the second form of musculoskeletal modeling, the same goal of finding optimal movement

patterns can be achieved in a matter of minutes. This is also a significant improvement in the second form of the ODSG process as compared to chapter 5. The primary reason for reduction in computational time in this study is the initial guess. Chapter 5 used a random initial guess, while this study used the initial motion as the initial guess since the objective is to find optimal movement pattern that is close to the original motion. Finding optimal movement patterns within a matter of minutes means that a patient or athlete can walk into a motion capture lab, have their movement data collected, and the optimized movement pattern can potentially be found, tested, and adjusted within an hour. Participant recruitment, especially for a multiple session study, is often seen as a bottleneck in experimental research. Our efficient methods solve this problem as they remove the need for multiple sessions, one to collect the data and one to test the optimized motion. From a clinical point of view, it saves patients multiple trips to the clinician increasing the likelihood of success of intervention and hence, increasing the clinical relevance. The secondary benefit to researchers is that the anthropometric measures and marker placement of the participants remain constant between the data collection and optimal movement testing phase, increasing scientific rigor.

Our study has a few limitations. First, since we had gait data from only four participants, external validity of our findings is greatly restricted. We found that even with a small sample size, multiple gait modifications lead to a decrease in the KAM (Fregly, 2008; Fregly et al., 2007; Guo et al., 2007). It is possible that other gait modifications that have been suggested in the literature are also capable in

achieving the same objective for certain individuals, but our small sample size did not allow for such findings. Second, we used the same foot contact model, scaled to each participant, rather than optimizing the parameters of the foot contact model to each participant. Even though it has been found that differences in foot contact models do not affect the simulations (Falisse et al., 2019), and another study has been done using the same foot contact model for multiple participants (Lin and Pandy, 2017), lack of participant specificity in the foot contact model can cause minor errors. This limitation can be addressed through an experimental validation study of our results. Third, we did not restrict the knee adduction angle of the participants based on their physical characteristics. Certain knee OA patients experience a change in the range of motion of knee adduction angle due to a degradation of the medial femoral condyle (Duffell et al., 2014). Since our study did not adjust for the range of motion of the knee adduction angle, certain movement patterns that we found might not be ideal for some patient's bone geometry. On the other hand, this change can be easily implemented at the clinical level based on the participant feedback, still within a clinically relevant time frame because of the computational efficiency. Fourth, since our models were driven by ideal torque actuators and not muscles, our study does not allow for understanding the behavior of the muscles to achieve the optimal movement. This limitation can be addressed by adding muscles in the model. Note that the aim of this study was to generate optimal gait patterns and test the efficiency of the methods, and muscles were not essential for this purpose. Nonetheless, the addition of muscles

can still help better understand the mechanism and design better rehabilitation protocols. Addition of muscles to the model would increase the time taken to generate the simulations, but it should still be within a clinically relevant time frame based on the fact that similar methods have been employed to generate gait simulations of a healthy individual using muscles as actuators (Falisse et al., 2019). Fifth, most of the kinematic changes observed in our study were in the coordinates of the affected leg (Fig. 6.2). This is primarily because the coordinates of the non-affected leg and the trunk were tracked at a higher weight than those of the affected leg. This was done to ensure that the optimal simulations do not look too different from the original gait patterns as patients prefer not to use them in social situations, which is the primary reason why trunk lean (Hunt et al., 2008), the most effective gait modification, is not widely popular. Our choice of different weights of the cost functions well suited our purpose, but further research is required to determine the best combination of weights of different terms in the cost function.

CHAPTER SEVEN

CONCLUSIONS AND FUTURE WORK

7.1. Conclusions

This work featured an advancement of the computational tools to generate simulations that address biomechanical needs of a variety of movements. In addition, chapter 2 enhanced our fundamental understanding of the role of residuals (errors) in a dynamic consistency of simulations and set forth guidelines that the simulation community can use to ensure that their simulations are within the limits of the laws of physics.

From the point of view of the optimal dynamic simulation generation (ODSG) process, this work made several improvements taking it from a researcher's tool that could be used only for a small set of movements and requires days to implement, to a tool that can be used on a variety of movements by the practitioners themselves. These advancements include addition of robotics-based concepts to enhance the dynamic consistency of simulations, addition of novel ways to enhance performance parameters, addition of goal-oriented cost functions to find simulations that achieve performance-injury prevention balance across multiple joints of the body, and finally increasing the computational efficiency to make the process fast enough to be clinically relevant.

Additionally, we tested the robustness of our methods for finding optimal movement patterns on a variety of movements like single-leg jump-landing, volleyball spiking, and pathological gait, addressing the biomechanical needs of both the upper and lower body. The variety of movements tested our system across both high-speed athletic movements and low-speed pathological

movements, and both aerial and grounded movements. Additionally, we also found the kinematic changes that help achieve the biomechanical needs. These kinematic changes can become the focus of rehabilitation or training protocols to help users learn the optimal movement patterns. We also determined the mechanism by which these kinematic changes elicit the changes in the biomechanics. We found that segments that are not even directly connected to the segment of interest could play a major role in addressing the biomechanical needs of the segment of interest. For example, in chapter 4, we found that the motion of the legs is critical to enhance the performance parameters at the wrist of the hitting hand and to reduce injury risk parameters at the shoulder. The knowledge of the mechanism allows clinicians, scientist, and practitioners to understand how the biomechanical parameters relate to the different segments of the body, identify the most important segments, and design appropriate training or rehabilitation protocols.

The results of chapter 6 showed that simulations of four different participants achieved the same biomechanical goals by employing four different kinematic strategies. These results highlight that a general pattern might not always work for everyone and provide evidence as to why gait modifications suggested in the literature to reduce the progression of knee osteoarthritis have largely failed. The ability of our methods to find participant-specific movement patterns greatly increases the robustness of our system. Additionally, the use of goal-oriented cost functions in chapter 4 provided evidence that our system can

also incorporate detailed needs of the participant. The design of the system allows the user to choose performance or injury prevention parameters that can be tailored to specific individuals.

Chapter 6 took the optimization process from taking multiple days to mere minutes. This is a significant advancement because clinicians can now use these methods to find optimal participant-specific movements in a clinically relevant time frame. For example, movement data from a participant can be collected in a motion capture lab, and the optimal movement pattern can be found and tested, and even adjusted and retested within about an hour.

7.2. Future Work

As with all research, our work also raises opportunity for improvement. First, the guidelines that we developed to assess the dynamic consistency of simulations only feature dynamic consistency related to model kinetics. Our guidelines could benefit from further refinements that add effects of residuals on model kinematics.

The biggest limitation of our work to finding optimal movement patterns was that we used torque driven simulations rather than muscle driven. This does not limit the ability of our methods to find optimal movement patterns but use of muscle driven models can greatly benefit the applicability of our methods as it can help practitioners identify the key muscles important to address the biomechanical needs in addition to the key kinematics and mechanism changes. A limitation of the faster form of finding optimal movement patterns used in this study is that it uses gradient-based optimization methods. These methods do not allow for goal-

oriented step functions in the cost function, the technique we employed to aid the optimization process to achieve the performance-injury prevention balance in chapter 4. This limitation can, however, be addressed by using a smooth function that imitates the step functions but can be used for gradient-based optimization (Dembia et al., 2021; Serrancoí et al., 2019). The best way to formulate and integrate these functions to the trajectory optimization-based framework used by the faster form of the ODSG process will require research. Another area that the ODSG process could benefit from is finding a way to appropriately weight the different terms in the cost functions. Lastly, we believe that our work is nearly ready to be used by practitioners but needs to be packaged in a user-friendly application or graphical user interface.

From an application point of view, our findings would benefit from an experimental validation. This would entail experimental studies of single-leg jump-landing, volleyball spiking, and gait of knee osteoarthritis patients that test the validity of the optimal movement patterns we found in this work. From the point of view of long-term application, our results would benefit from studies aimed to find the best ways to learn the new movement patterns. The key kinematics and mechanism changes found in our study can act as guide to develop new training and rehabilitation protocols that could teach the optimal movement patterns. Some of the techniques that could also be employed to teach the optimal patterns are video-based implicit learning (Farrow and Abernethy, 2002; Williams et al., 2002), muscular training (Staynor et al., 2017; Weir, 2014; Weir et al., 2014), real-time

feedback-based learning (Barrios et al., 2010; Pizzolato et al., 2017), and large-scale interventions studies built on sound mechanics and behavior change principles (Donnelly et al., 2020).

LIST OF REFERENCES

Baliunas, A.J., Hurwitz, D.E., Ryals, A.B., Karrar, A., Case, J.P., Block, J.A., Andriacchi, T.P., 2002. Increased knee joint loads during walking are present in subjects with knee osteoarthritis. *Osteoarthritis and Cartilage* 10, 573-579.

Barrios, J.A., Crossley, K.M., Davis, I.S., 2010. Gait retraining to reduce the knee adduction moment through real-time visual feedback of dynamic knee alignment. *Journal of biomechanics* 43, 2208-2213.

Besier, T.F., Lloyd, D.G., Cochrane, J.L., Ackland, T.R., 2001. External loading of the knee joint during running and cutting maneuvers. *Medicine & Science in Sports & Exercise* 33, 1168-1175.

Besier, T.F., Sturnieks, D.L., Alderson, J.A., Lloyd, D.G., 2003. Repeatability of gait data using a functional hip joint centre and a mean helical knee axis. *Journal of biomechanics* 36, 1159-1168.

Betts, J.T., 2010. Practical methods for optimal control and estimation using nonlinear programming. SIAM.

Bishop, R.D., Hay, J.G., 1979. Basketball: the mechanics of hanging in the air. *Medicine and science in sports* 11, 274-277.

Briner, W.W., Kacmar, L., 1997. Common Injuries in Volleyball. *Sports Medicine* 24, 65-71.

Brophy, R.H., Wright, R.W., Matava, M.J., 2009. Cost Analysis of Converting from Single-Bundle to Double-Bundle Anterior Cruciate Ligament Reconstruction. *The American Journal of Sports Medicine* 37, 683-687.

Brown, J.R., Alsarraf, B.J., Waller, M., Eisenman, P., Hicks-Little, C.A., 2014a. Rotational Angles and Velocities During Down the Line and Diagonal Across Court Volleyball Spikes. *International Journal of Kinesiology & Sports Science* 2, 1-8.

Brown, S.R., Brughelli, M., Hume, P.A., 2014b. Knee Mechanics During Planned and Unplanned Sidestepping: A Systematic Review and Meta-Analysis. *Sports Medicine* 44, 1573-1588.

Cerulli, G., Benoit, D.L., Lamontagne, M., Caraffa, A., Liti, A., 2003. In vivo anterior cruciate ligament strain behaviour during a rapid deceleration movement: case report. *Knee Surgery, Sports Traumatology, Arthroscopy* 11, 307-311.

Challoumas, D., Stavrou, A., Dimitrakakis, G., 2017. The volleyball athlete's shoulder: biomechanical adaptations and injury associations. *Sports Biomechanics* 16, 220-237.

Chaudhari, A.M., Hearn, B.K., Andriacchi, T.P., 2005. Sport-dependent variations in arm position during single-limb landing influence knee loading: implications for anterior cruciate ligament injury. *The American journal of sports medicine* 33, 824-830.

Chinnasee, C., Weir, G., Sasimontongkul, S., Alderson, J., Donnelly, C., 2018. A Biomechanical Comparison of Single-Leg Landing and Unplanned Sidestepping. *Int J Sports Med* 39, 636-645.

Cochrane, J.L., Lloyd, D.G., Besier, T.F., Elliott, B.C., Doyle, T.L., Ackland, T.R., 2010. Training affects knee kinematics and kinetics in cutting maneuvers in sport. *Medicine & Science in Sports & Exercise* 42, 1535-1544.

Cochrane, J.L., Lloyd, D.G., Butfield, A., Seward, H., McGivern, J., 2007. Characteristics of anterior cruciate ligament injuries in Australian football. *Journal of Science and Medicine in Sport* 10, 96-104.

Damsgaard, M., Rasmussen, J., Christensen, S.T., Surma, E., de Zee, M., 2006. Analysis of musculoskeletal systems in the AnyBody Modeling System. *Simulation Modelling Practice and Theory* 14, 1100-1111.

de Leva, P., 1996. Adjustments to Zatsiorsky-Seluyanov's segment inertia parameters. *Journal of biomechanics* 29, 1223-1230.

Delp, S.L., Anderson, F.C., Arnold, A.S., Loan, P., Habib, A., John, C.T., Guendelman, E., Thelen, D.G., 2007. OpenSim: Open-Source Software to Create and Analyze Dynamic Simulations of Movement. *IEEE Transactions on Biomedical Engineering* 54, 1940-1950.

Delp, S.L., Loan, J.P., Hoy, M.G., Zajac, F.E., Topp, E.L., Rosen, J.M., 1990. An interactive graphics-based model of the lower extremity to study orthopaedic surgical procedures. *IEEE Transactions on Biomedical Engineering* 37, 757-767.

Dembia, C.L., Bianco, N.A., Falisse, A., Hicks, J.L., Delp, S.L., 2019. OpenSim Moco: Musculoskeletal optimal control. *bioRxiv*, 839381.

Dembia, C.L., Bianco, N.A., Falisse, A., Hicks, J.L., Delp, S.L., 2021. OpenSim Moco: Musculoskeletal optimal control. *PLOS Computational Biology* 16, e1008493.

Dempsey, A.R., Elliott, B.C., Munro, B.J., Steele, J.R., Lloyd, D.G., 2012. Whole body kinematics and knee moments that occur during an overhead catch and landing task in sport. *Clinical Biomechanics* 27, 466-474.

Dempsey, A.R., Lloyd, D.G., Elliott, B.C., Steele, J.R., Munro, B.J., Russo, K.A., 2007. The effect of technique change on knee loads during sidestep cutting. *Medicine & Science in Sports & Exercise* 39, 1765-1773.

Donnelly, C.J., Chinnasee, C., Weir, G., Sasimontongkul, S., Alderson, J., 2017. Joint dynamics of rear- and fore-foot unplanned sidestepping. *Journal of Science and Medicine in Sport* 20, 32-37.

Donnelly, C.J., Elliott, B.C., Ackland, T.R., Doyle, T.L.A., Beiser, T.F., Finch, C.F., Cochrane, J.L., Dempsey, A.R., Lloyd, D.G., 2012a. An Anterior Cruciate Ligament Injury Prevention Framework: Incorporating the Recent Evidence. *Research in Sports Medicine* 20, 239-262.

Donnelly, C.J., Elliott, B.C., Doyle, T.L.A., Finch, C.F., Dempsey, A.R., Lloyd, D.G., 2012b. Changes in knee joint biomechanics following balance and technique training and a season of Australian football. *British Journal of Sports Medicine* 46, 917.

Donnelly, C.J., Jackson, B.S., Gucciardi, D.F., Reinbolt, J., 2020. Biomechanically-Informed Training: The Four Pillars for Knee and ACL Injury Prevention Built Upon Behavior Change and Motivation Principles. *Applied Sciences* 10, 4470.

Donnelly, C.J., Jackson, C., Weir, G., Alderson, J., Robinson, M.A., 2021. Prescribing joint co-ordinates during model preparation in OpenSim improves lower limb unplanned sidestepping kinematics. *J Sci Med Sport* 24, 159-163.

Donnelly, C.J., Lloyd, D.G., Elliott, B.C., Reinbolt, J.A., 2012c. Optimizing whole-body kinematics to minimize valgus knee loading during sidestepping: Implications for ACL injury risk. *Journal of biomechanics* 45, 1491-1497.

Dramis, A., Pimpalnerkar, A., 2005. Suprascapular neuropathy in volleyball players. *Acta Orthop Belg* 71, 269-272.

Duffell, L.D., Mushtaq, J., Masjedi, M., Cobb, J.P., 2014. The knee adduction angle of the osteo-arthritic knee: A comparison of 3D supine, static and dynamic alignment. *The Knee* 21, 1096-1100.

Dunn, W.R., Spindler, K.P., 2010. Predictors of Activity Level 2 Years after Anterior Cruciate Ligament Reconstruction (ACLR): A Multicenter Orthopaedic Outcomes Network (MOON) ACLR Cohort Study. *The American Journal of Sports Medicine* 38, 2040-2050.

Edmonds, D.W., McConnell, J., Ebert, J.R., Ackland, T.R., Donnelly, C.J., 2016. Biomechanical, neuromuscular and knee pain effects following therapeutic knee taping among patients with knee osteoarthritis during walking gait. *Clinical Biomechanics* 39, 38-43.

Eerkes, K., 2012. Volleyball Injuries. *Current Sports Medicine Reports* 11, 251-256.

Falisse, A., Serrancoí, G., Dembia, C.L., Gillis, J., Jonkers, I., De Groote, F., 2019. Rapid predictive simulations with complex musculoskeletal models suggest that diverse healthy and pathological human gaits can emerge from similar control strategies. *Journal of The Royal Society Interface* 16, 20190402.

Farrow, D., Abernethy, B., 2002. Can anticipatory skills be learned through implicit video based perceptual training? *Journal of Sports Sciences* 20, 471-485.

Fortin-Guichard, D., Laflamme, V., Julien, A.-S., Trottier, C., Grondin, S., 2020. Decision-making and dynamics of eye movements in volleyball experts. *Scientific Reports* 10, 17288.

Fregly, B.J., 2008. Computational assessment of combinations of gait modifications for knee osteoarthritis rehabilitation. *IEEE transactions on bio-medical engineering* 55, 2104-2106.

Fregly, B.J., Besier, T.F., Lloyd, D.G., Delp, S.L., Banks, S.A., Pandy, M.G., D'Lima, D.D., 2012. Grand challenge competition to predict in vivo knee loads. *Journal of Orthopaedic Research* 30, 503-513.

Fregly, B.J., Reinbolt, J.A., Chmielewski, T.L., 2008. Evaluation of a patient-specific cost function to predict the influence of foot path on the knee adduction torque during gait. *Computer methods in biomechanics and biomedical engineering* 11, 63-71.

Fregly, B.J., Reinbolt, J.A., Rooney, K.L., Mitchell, K.H., Chmielewski, T.L., 2007. Design of patient-specific gait modifications for knee osteoarthritis rehabilitation. *IEEE transactions on bio-medical engineering* 54, 1687-1695.

Goffe, W.L., Ferrier, G.D., Rogers, J., 1994. Global optimization of statistical functions with simulated annealing. *Journal of Econometrics* 60, 65-99.

Guo, M., Axe, M.J., Manal, K., 2007. The influence of foot progression angle on the knee adduction moment during walking and stair climbing in pain free individuals with knee osteoarthritis. *Gait & Posture* 26, 436-441.

Gupta, D., Donnelly, C.J., Neptune, R.R., Abraham, L.D., Jensen, J.L., Reinbolt, J.A., 2018a. Use of musculoskeletal modeling to find the balance between performance and injury prevention in sports – A proof of concept, 36th International Conference on Biomechanics in Sports, Auckland, New Zealand.

Gupta, D., Donnelly, C.J., Reinbolt, J.A., 2019a. Reasonable simulations depend on relationships between calculated residual forces and moments: Implications for residual threshold limits., 17th International Symposium on Computer Simulation in Biomechanics., Canmore, Canada, pp. 55-56.

Gupta, D., Donnelly, C.J., Reinbolt, J.A., 2020. Optimizing whole-body kinematics using OpenSim Moco to reduce peak non-sagittal plane knee loads and ACL injury risk during single leg jump landing, 44th Annual Meeting of the American Society of Biomechanics, p. 129.

Gupta, D., Jensen, J.L., Abraham, L.D., 2015. Biomechanical study of mid-flight body segment action and its effect on hang-time for volleyball spike jumps, 33rd International Conference on Biomechanics in Sports, Poitiers, France.

Gupta, D., Jensen, J.L., Abraham, L.D., 2021. Biomechanics of hang-time in volleyball spike jumps. *Journal of biomechanics* 121, 110380.

Gupta, D., Jensen, J.L., Donnelly, C.J., Reinbolt, J.A., 2019b. Synergistic trunk dynamics reduces risk of shoulder injury during volleyball hitting., 27th Congress of the International Society of Biomechanics, Calgary, Canada, p. 100.

Gupta, D., Reinbolt, J.A., Jensen, J.L., Donnelly, C.J., 2018b. Optimizing whole body kinematics to reduce peak non-sagittal plane knee loads during single leg jump landing task to reduce risk of ACL injury, 42nd Annual Meeting of the American Society of Biomechanics, Rochester, Minnesota, USA.

Hamner, S.R., Seth, A., Delp, S.L., 2010. Muscle contributions to propulsion and support during running. *Journal of biomechanics* 43, 2709-2716.

Heidari, B., 2011. Knee osteoarthritis prevalence, risk factors, pathogenesis and features: Part I. *Caspian journal of internal medicine* 2, 205-212.

Hewett, T.E., Myer, G.D., Ford, K.R., 2006. Anterior cruciate ligament injuries in female athletes: Part 1, mechanisms and risk factors. *The American journal of sports medicine* 34, 299-311.

Hicks, J.L., Uchida, T.K., Seth, A., Rajagopal, A., Delp, S.L., 2015. Is My Model Good Enough? Best Practices for Verification and Validation of Musculoskeletal Models and Simulations of Movement. *Journal of biomechanical engineering* 137, 020905-020905-020924.

Holzbaur, K.R., Murray, W.M., Delp, S.L., 2005. A model of the upper extremity for simulating musculoskeletal surgery and analyzing neuromuscular control. *Annals of biomedical engineering* 33, 829-840.

Hunt, M.A., Birmingham, T.B., Bryant, D., Jones, I., Giffin, J.R., Jenkyn, T.R., Vandervoort, A.A., 2008. Lateral trunk lean explains variation in dynamic knee joint

load in patients with medial compartment knee osteoarthritis. *Osteoarthritis and Cartilage* 16, 591-599.

Igielska-Bela, B., Baczkowski, B., Flisikowski, K., 2020. Shoulder ultrasound in the diagnosis of the suprascapular neuropathy in athletes. *Open Medicine* 15, 147-151.

Jackson, J.N., Hass, C.J., Fregly, B.J., 2016. Development of a Subject-Specific Foot-Ground Contact Model for Walking. *Journal of biomechanical engineering* 138.

James, L.P., Kelly, V.G., Beckman, E.M., 2014. Injury Risk Management Plan for Volleyball Athletes. *Sports Medicine* 44, 1185-1195.

Kramer, L.C., 2010. Understanding and Preventing Noncontact ACL Injuries. *Athletic Training and Sports Health Care* 2, 43-44.

Kugler, A., Krüger-Franke, M., Reininger, S., Trouillier, H.H., Rosemeyer, B., 1996. Muscular imbalance and shoulder pain in volleyball attackers. *British Journal of Sports Medicine* 30, 256.

Lajtai, G., Wieser, K., Ofner, M., Raimann, G., Aitzetmüller, G., Jost, B., 2012. Electromyography and nerve conduction velocity for the evaluation of the infraspinatus muscle and the suprascapular nerve in professional beach volleyball players. *The American Journal of Sports Medicine* 40, 2303-2308.

Landry, S.C., McKean, K.A., Hubley-Kozey, C.L., Stanish, W.D., Deluzio, K.J., 2007. Knee biomechanics of moderate OA patients measured during gait at a self-selected and fast walking speed. *Journal of biomechanics* 40, 1754-1761.

Lawrence, R.C., Felson, D.T., Helmick, C.G., Arnold, L.M., Choi, H., Deyo, R.A., Gabriel, S., Hirsch, R., Hochberg, M.C., Hunder, G.G., Jordan, J.M., Katz, J.N., Kremers, H.M., Wolfe, F., 2008. Estimates of the prevalence of arthritis and other rheumatic conditions in the United States: Part II. *Arthritis & Rheumatism* 58, 26-35.

Leonard, J., Hutchinson, M.R., 2010. Shoulder injuries in skeletally immature throwers: review and current thoughts. *British Journal of Sports Medicine* 44, 306.

Leong, H.T., Ng, G.Y.-f., Fu, S.N., 2017. Effects of scapular taping on the activity onset of scapular muscles and the scapular kinematics in volleyball players with rotator cuff tendinopathy. *Journal of science and medicine in sport* 20, 555-560.

Lespasio, M.J., Piuze, N.S., Husni, M.E., Muschler, G.F., Guarino, A., Mont, M.A., 2017. Knee Osteoarthritis: A Primer. *The Permanente journal* 21.

Lin, Y.-C., Pandy, M.G., 2017. Three-dimensional data-tracking dynamic optimization simulations of human locomotion generated by direct collocation. *Journal of biomechanics* 59, 1-8.

Losina, E., Paltiel, A.D., Weinstein, A.M., Yelin, E., Hunter, D.J., Chen, S.P., Klara, K., Suter, L.G., Solomon, D.H., Burbine, S.A., Walensky, R.P., Katz, J.N., 2015. Lifetime medical costs of knee osteoarthritis management in the United States: impact of extending indications for total knee arthroplasty. *Arthritis care & research* 67, 203-215.

Lynn, S.K., Kajaks, T., Costigan, P.A., 2008. The effect of internal and external foot rotation on the adduction moment and lateral–medial shear force at the knee during gait. *Journal of Science and Medicine in Sport* 11, 444-451.

MacDonald, K., Bahr, R., Baltich, J., Whittaker, J.L., Meeuwisse, W.H., 2017. Validation of an inertial measurement unit for the measurement of jump count and height. *Physical Therapy in Sport* 25, 15-19.

Manal, K., Gardinier, E., Buchanan, T.S., Snyder-Mackler, L., 2015. A more informed evaluation of medial compartment loading: the combined use of the knee adduction and flexor moments. *Osteoarthritis and Cartilage* 23, 1107-1111.

Markolf, K.L., Burchfield, D.M., Shapiro, M.M., Shepard, M.F., Finerman, G.A., Slauterbeck, J.L., 1995. Combined knee loading states that generate high anterior cruciate ligament forces. *Journal of Orthopaedic Research* 13, 930-935.

McConnell, J., Donnelly, C., Hamner, S., Dunne, J., Besier, T., 2011. Effect of shoulder taping on maximum shoulder external and internal rotation range in uninjured and previously injured overhead athletes during a seated throw. *Journal of Orthopaedic Research* 29, 1406-1411.

McLean, S.G., Huang, X., van den Bogert, A.J., 2005. Association between lower extremity posture at contact and peak knee valgus moment during sidestepping: implications for ACL injury. *Clinical Biomechanics* 20, 863-870.

Mihata, T., McGarry, M.H., Kinoshita, M., Lee, T.Q., 2010. Excessive glenohumeral horizontal abduction as occurs during the late cocking phase of the throwing motion can be critical for internal impingement. *The American journal of sports medicine* 38, 369-374.

Mirhassan Zadeh Kuhkamar, M., Hadadnezhad, M., Khaleghi Tazji, M., 2020. The effect of eight weeks' scapular focused training on pain, proprioception, scapular kinematics and upper extremity performance in male volleyball players with shoulder impingement syndrome: a randomized clinical trial study. *Medical Journal of Tabriz University of Medical Sciences and Health Services* 42, 466-475.

Morgan, K.D., Donnelly, C.J., Reinbolt, J.A., 2014. Elevated gastrocnemius forces compensate for decreased hamstrings forces during the weight-acceptance phase of single-leg jump landing: implications for anterior cruciate ligament injury risk. *Journal of Biomechanics* 47, 3295-3302.

Myer, G.D., Ford, K.R., Palumbo, O.P., Hewett, T.E., 2005. Neuromuscular training improves performance and lower-extremity biomechanics in female athletes. *The Journal of Strength & Conditioning Research* 19, 51-60.

Ogaya, S., Naito, H., Iwata, A., Higuchi, Y., Fuchioka, S., Tanaka, M., 2014. Knee adduction moment and medial knee contact force during gait in older people. *Gait Posture* 40, 341-345.

Pizzolato, C., Reggiani, M., Saxby, D.J., Ceseracciu, E., Modenese, L., Lloyd, D.G., 2017. Biofeedback for Gait Retraining Based on Real-Time Estimation of Tibiofemoral Joint Contact Forces. *IEEE transactions on neural systems and rehabilitation engineering : a publication of the IEEE Engineering in Medicine and Biology Society* 25, 1612-1621.

Reeser, J.C., Joy, E.A., Porucznik, C.A., Berg, R.L., Colliver, E.B., Willick, S.E., 2010. Risk factors for volleyball-related shoulder pain and dysfunction. *Pm&r* 2, 27-36.

Reinbolt, J.A., Donnelly, C.J., Year Predicting ground reactions during single-leg landings using zero-moment point. In 26th Congress of the International Society of Biomechanics. Brisbane, Australia.

Reinbolt, J.A., Donnelly, C.J., 2017b. Predicting ground reactions during single-leg landings using zero-moment point., 26th Congress of the International Society of Biomechanics.

Reinbolt, J.A., Seth, A., Delp, S.L., 2011. Simulation of human movement: applications using OpenSim. *Procedia IUTAM* 2, 186-198.

Robbins, S.M.K., Maly, M.R., 2009. The effect of gait speed on the knee adduction moment depends on waveform summary measures. *Gait & Posture* 30, 543-546.

Saini, N., Price, E., Tallamraju, R., Enficiaud, R., Ludwig, R., Martinovic, I., Ahmad, A., Black, M.J., Year Markerless outdoor human motion capture using multiple autonomous micro aerial vehicles. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*.

Schache, A.G., Fregly, B.J., Crossley, K.M., Hinman, R.S., Pandy, M.G., 2008. The effect of gait modification on the external knee adduction moment is reference frame dependent. *Clinical Biomechanics* 23, 601-608.

Seminati, E., Marzari, A., Vacondio, O., Minetti, A.E., 2015. Shoulder 3D range of motion and humerus rotation in two volleyball spike techniques: injury prevention and performance. *Sports biomechanics* 14, 216-231.

Serrancolí, G., Falisse, A., Dembia, C., Vantilt, J., Tanghe, K., Lefeber, D., Jonkers, I., De Schutter, J., De Groote, F., 2019. Subject-exoskeleton contact model calibration leads to accurate interaction force predictions. *IEEE Transactions on Neural Systems and Rehabilitation Engineering* 27, 1597-1605.

Serrien, B., Ooijen, J., Goossens, M., Baeyens, J.-P., 2016. A motion analysis in the volleyball spike—part 1: three dimensional kinematics and performance. *Int J Hum Mov Sports Sci* 4, 70-82.

Sherman, M.A., Seth, A., Delp, S.L., 2011. Simbody: multibody dynamics for biomedical research. *Procedia Iutam* 2, 241-261.

Shih, Y.-F., Wang, Y.-C., 2019. Spiking Kinematics in Volleyball Players With Shoulder Pain. *Journal of athletic training* 54, 90-98.

Staynor, J.M., Byrne, S.D., Alderson, J.A., Donnelly, C.J., 2019. The applied impact of 'naïve' statistical modelling of clustered observations of motion data in injury biomechanics research. *Journal of science and medicine in sport* 22, 420-424.

Staynor, J.M.D., Nicholas, J.C., Weir, G., Alderson, J.A., Donnelly, C.J., 2017. Targeting associated mechanisms of anterior cruciate ligament injury in female community-level athletes. *Sports Biomechanics* 16, 501-513.

Stearne, S.M., Alderson, J.A., Green, B.A., Donnelly, C.J., Rubenson, J., 2014. Joint kinetics in rearfoot versus forefoot running: implications of switching technique. *Medicine & Science in Sports & Exercise* 46, 1578-1587.

Thelen, D.G., Anderson, F.C., 2006. Using computed muscle control to generate forward dynamic simulations of human walking from experimental data. *Journal of biomechanics* 39, 1107-1115.

Topputo, F., Zhang, C., 2014. Survey of Direct Transcription for Low-Thrust Space Trajectory Optimization with Applications. *Abstract and Applied Analysis* 2014, 851720.

Trepczynski, A., Kutzner, I., Bergmann, G., Taylor, W.R., Heller, M.O., 2014. Modulation of the relationship between external knee adduction moments and medial joint contact forces across subjects and activities. *Arthritis & rheumatology (Hoboken, N.J.)* 66, 1218-1227.

Uhlrich, S.D., Kolesar, J.A., Kidziński, Ł., Boswell, M.A., Silder, A., Gold, G.E., Delp, S.L., Beaupre, G.S., 2020. Personalization improves the biomechanical efficacy of foot progression angle modifications in individuals with medial knee osteoarthritis. *medRxiv*, 2020.2012.2015.20248220.

Ulrich, B., Cosendey, K., Jolles, B.M., Favre, J., 2020. Decreasing the ambulatory knee adduction moment without increasing the knee flexion moment individually through modifications in footprint parameters: A feasibility study for a dual kinetic change in healthy subjects. *Journal of biomechanics* 111, 110004.

Utturkar, G.M., Iribarra, L.A., Taylor, K.A., Spritzer, C.E., Taylor, D.C., Garrett, W.E., DeFrate, L.E., 2013. The Effects of a Valgus Collapse Knee Position on In Vivo ACL Elongation. *Annals of biomedical engineering* 41, 123-130.

Vukobratović, M., Borovac, B., 2004. Zero-moment point—thirty five years of its life. *International journal of humanoid robotics* 1, 157-173.

Walter, J.P., D'Lima, D.D., Colwell, C.W., Fregly, B.J., 2010. Decreased knee adduction moment does not guarantee decreased medial contact force during gait. *Journal of Orthopaedic Research* 28, 1348-1354.

Wang, H., Cochrane, T., 2001. A descriptive epidemiological study of shoulder injury in top level English male volleyball players. *International journal of sports medicine* 22, 159-163.

Weir, G., 2014. A 25-week biomechanically informed two phase injury prevention training program: Implications for ACL injury risk among elite female hockey players. *Preventing anterior cruciate ligament injuries in sport: a biomechanically informed approach to training*.

Weir, G., Cantwell, D., Alderson, J., Elliott, B.C., Donnelly, C.J., 2014. Changes in support moment and muscle activation following hip and trunk neuromuscular training: The hip and ACL injury risk, 32nd International Conference of Biomechanics in Sports, Johnson City, Tennessee, USA.

Williams, A.M., Ward, P., Knowles, J.M., Smeeton, N.J., 2002. Anticipation skill in a real-world task: measurement, training, and transfer in tennis. *Journal of Experimental Psychology: Applied* 8, 259.

Winby, C.R., Lloyd, D.G., Besier, T.F., Kirk, T.B., 2009. Muscle and external load contribution to knee joint contact loads during normal gait. *Journal of biomechanics* 42, 2294-2300.

- Winter, D.A., 2009. Biomechanics and motor control of human movement. John Wiley & Sons.
- Xiang, Y., Arora, J.S., Abdel-Malek, K., 2010. Physics-based modeling and simulation of human walking: a review of optimization-based and other approaches. *Structural and Multidisciplinary Optimization* 42, 1-23.
- Xiang, Y., Arora, J.S., Rahmatalla, S., Abdel-Malek, K., 2009. Optimization-based dynamic human walking prediction: One step formulation. *International Journal for Numerical Methods in Engineering* 79, 667-695.
- Zazulak, B.T., Hewett, T.E., Reeves, N.P., Goldberg, B., Cholewicki, J., 2007. Deficits in neuromuscular control of the trunk predict knee injury risk: prospective biomechanical-epidemiologic study. *The American journal of sports medicine* 35, 1123-1130.
- Zhang, Y., Jordan, J.M., 2010. Epidemiology of osteoarthritis. *Clinics in geriatric medicine* 26, 355-369.
- Zhao, D., Banks, S.A., D'Lima, D.D., Colwell, C.W., Jr., Fregly, B.J., 2007. In vivo medial and lateral tibial loads during dynamic and high flexion activities. *Journal of orthopaedic research : official publication of the Orthopaedic Research Society* 25, 593-602.

VITA

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