Numerical modelling of the shoulder for clinical applications

BY PHILIPPE FAVRE*, JESS G. SNEDEKER AND CHRISTIAN GERBER

Laboratory for Orthopaedic Research, Department of Orthopaedics, Balgrist, University of Zurich, Forchstrasse 340, 8008 Zurich, Switzerland

Research activity involving numerical models of the shoulder is dramatically increasing, driven by growing rates of injury and the need to better understand shoulder joint pathologies to develop therapeutic strategies. Based on the type of clinical question they can address, existing models can be broadly categorized into three groups: (i) rigid body models that can simulate kinematics, collisions between entities or wrapping of the muscles over the bones, and which have been used to investigate joint kinematics and ergonomics, and are often coupled with (ii) muscle force estimation techniques, consisting mainly of optimization methods and electromyography-driven models, to simulate muscular action and joint reaction forces to address issues in joint stability, muscular rehabilitation or muscle transfer, and (iii) deformable models that account for stress–strain distributions in the component structures to study articular degeneration, implant failure or muscle/tendon/bone integrity. The state of the art in numerical modelling of the shoulder is reviewed, and the advantages, limitations and potential clinical applications of these modelling approaches are critically discussed. This review concentrates primarily on muscle force estimation modelling, with emphasis on a novel muscle recruitment paradigm, compared with traditionally applied optimization methods. Finally, the necessary benchmarks for validating shoulder models, the emerging technologies that will enable further advances and the future challenges in the field are described.

Keywords: shoulder biomechanics; computer/numerical modelling; glenohumeral joint; muscle force estimation; rigid body model; finite element

1. Introduction

(a) Increasing interest in shoulder modelling

Historically, in orthopaedics, most numerical simulations have focused on the hip and the knee, with fewer on the shoulder. From a clinical perspective, the hip and knee have largely occupied the interests of clinical and industrial researchers because the vast majority of joint replacements are performed at these joints.
From a modelling standpoint, the complexity of the shoulder joint itself may be a disincentive to modellers, who have to cope with intricate active and passive stabilizing mechanisms and an extremely large range of joint motions (Hogfors et al. 1995). Upper extremity motions are by necessity more variable than the locomotive movements of the lower limb (a well-defined cyclic motion), and while a two-dimensional analysis of gait can reasonably characterize leg kinematics, such a simplified treatment of the shoulder is inadequate (Rau et al. 2000).

Shoulder problems are gaining research interest as 20–30 per cent of the population suffer from shoulder pain and 8.8 per cent suffer functional impairment (Lock et al. 1999; Makela et al. 1999). Furthermore, many major clinical challenges of shoulder orthopaedics have proven to be persistent, and a need for deeper understanding of shoulder pathology and treatment has become clear. On the modelling side, lessons learned from other joints can now be applied to the shoulder, and improvements in software and computational power have facilitated the building and solving of ever more complex models. All these factors have driven the exponential increase in the number of publications involving numerical models of the shoulder (figure 1), the most clinically relevant of which we review here.

(b) Essential clinical issues with potential to be addressed using models

Among the many shoulder problems encountered in daily clinical practice, several concerns are of particular interest to the modeller. First, they correspond to some of the most challenging issues in shoulder orthopaedics. Second, numerical simulations offer unique potential to improve their treatment.
(i) Glenohumeral instability

The glenohumeral joint is the most frequently dislocated major joint of the body, affecting at least 1.7 per cent of people in the course of their lifetime (Hovelius 1982). The contribution of the glenohumeral surface shape, capsule and ligaments to stability has been widely studied, although glenohumeral joint stability is primarily ensured by coordination of muscular actions (Lippitt & Matsen 1993; Veeger & van der Helm 2007). This is especially complex, as some muscles may act as stabilizers, while others rather tend to destabilize the joint, depending on joint position (van der Helm 1994a; McMahon & Lee 2002; Werner et al. 2007; Favre et al. 2009). Our present knowledge fails to explain many cases of instability, owing to insufficient understanding of how the muscles simultaneously move the humerus and prevent glenohumeral dislocation (Kronberg et al. 1991; McMahon & Lee 2002; Veeger & van der Helm 2007). Here, muscle force estimation models can be considerably helpful in studying active stabilization mechanisms. Rigid body or deformable models can be used to assess the influence of passive stabilizers and joint conformity in more depth.

(ii) Rotator cuff tears

The muscles of the rotator cuff maintain joint stability by pulling the humeral head into the glenoid socket. Tears of the rotator cuff tendons are common and have been shown to be present in over 50 per cent of asymptomatic people above the age of 60 (Sher et al. 1995), reflecting accumulated damage over the course of a lifetime. These tears may progress to massive, symptomatic tears, eventually leading to irreversible changes in the physiology of the muscle and tendon (Gerber et al. 2004), making surgical repair difficult. Torn cuff tendons can lead to pain, instability, dysfunction and osteoarthritis, and in the worst cases can degenerate to cuff tear arthropathy, in which the humeral head collapses (Neer et al. 1983). The pathogenesis of rotator cuff tears remains unclear, and the best treatment for this common disorder remains a source of debate (Williams et al. 2004). The evolution to a symptomatic tear is not well understood, and although many other factors are involved (vascular, genetic, etc.), finite-element (FE) analyses can provide first insight into tendon-loading patterns (Luo et al. 1998; Wakabayashi et al. 2003; Sano et al. 2006) or could give guidelines to optimize the mechanics of tendon repair. Interestingly, the functional deficits associated with rotator cuff tears are highly variable among patients, varying from normal range of motion to pseudoparalysis, indicating that some patients are able to cope with the torn muscles, while others cannot. Here, muscle force estimation models could help us to understand how compensation involving the remaining viable muscles occurs and to define new rehabilitation strategies.

(iii) Shoulder arthroplasty

The number of partial and total shoulder replacements remains relatively small in comparison with that for the hip or knee, but has tripled in just 10 years in the USA, reaching 29 000 partial and total shoulder replacements in 2004 (Kozak et al. 2006). The two major complications associated with joint replacement are loosening of the glenoid component and joint instability (Franklin et al. 1988; Wirth & Rockwood 1996).
Although the aetiology of glenoid loosening is not yet fully understood, it is generally believed to have several potential (and possibly interrelated) sources, notably implant design, implant wear and particle formation, surgical technique, poor bone quality and eccentric implant loading. Eccentric loading can be due to migration of the humeral head (Franklin et al. 1988) or disadvantageous implant positioning (Nyffeler et al. 2006). In their ability to explore mechanical phenomena, FE simulations offer potential to understand these issues.

As with the normal glenohumeral joint, instability of the prosthetic joint is also a primary concern. Because stability of the shoulder depends so heavily on the active musculature, muscle force estimation models may improve our understanding of the stability changes induced by an implant. Constrained devices such as the reverse prosthesis (in which the ball is transposed to the scapula and the socket to the humerus) provide increased intrinsic stability, but they have been associated with higher rates of surgical revision (Matsen et al. 2007). Moreover, the geometric and kinematic changes induced by the reverse design present many questions to be investigated (Boileau et al. 2005), and rigid body models may provide a tool for investigation. Generally, models may facilitate our quest for increased implant longevity by helping the surgeon in choosing an appropriate size, type and position of the prosthesis and guide in optimizing soft tissue tension and force balance.

(iv) Tendon transfer

Muscle transfer represents a viable treatment option to restore the lost function in a variety of difficult shoulder issues. The anatomical insertion of a functioning muscle is detached and transferred to a different location to fulfil a new role and restore a lost function. For instance, the latissimus dorsi transfer can restore external rotation in the case of irreparable rotator cuff tears (Gerber 1992), or be further combined with arthroplasty (Gerber et al. 2007). However, the clinical outcome of muscle transfers is still difficult to predict, and the biomechanical implications of such procedures are only beginning to be understood (Magermans et al. 2004a,b; Favre et al. 2008a). Rigid body models simulating muscle wrapping can provide first information on the muscle path and moment arm of the transferred muscle. Muscle force estimation models can then help in understanding how the changes induced by the transferred muscle influence the distribution of muscle forces over the whole joint. Generally, simulations should provide guidelines (choice of muscle to transfer, optimal insertion site and muscle training) to maximize the functional potential.

2. Numerical models of the shoulder

Simulations performed with numerical models allow investigation of aspects that are otherwise difficult or impossible to quantify, overcoming technical limits (deterioration of tissues, adequate placement of sensors, etc.) and ethical limits (invasiveness and short supply of specimens) on direct in vivo or in vitro measurements.

Depending on the aspect of shoulder function to be investigated, various modelling approaches can be selected. Because the clinical question generally dictates the kind of model to be used, in the current review we categorize the models based on the type of output they generate, and thus the type of clinical question they...
can address (table 1). This classification is not exhaustive, largely allows for overlapping between categories and focuses on the clinical issues described above. Accordingly, the available models can be broadly categorized into three main groups: (i) rigid body models that can simulate kinematics, collisions between entities or wrapping of the muscles over the bones, and which have been used to investigate joint kinematics and ergonomics, and have very often been coupled with (ii) muscle force estimation techniques, consisting mainly of optimization methods and electromyography (EMG)-driven models, to simulate muscular action (inverse dynamics) and joint reaction forces to address issues in joint stability, muscular rehabilitation or muscle transfer, and (iii) deformable models that account for stress–strain distributions in the component structures, and which can be used to study articular degeneration, implant failure or muscle integrity. This review does not intend to provide an exhaustive list of all published shoulder models but points out several key models that have been specifically tailored to address clinical questions.

(a) Rigid body models

Rigid body models idealize a system as consisting of solid bodies connected by kinematic constraints, and in which deformations of the bodies are neglected.
In applying this approach to the shoulder, the bones are represented as rigid segments, and the muscles as adjustable length segments that link their origin and insertion. Kinematics, collisions between entities or wrapping of the muscles over the bones can be simulated. Because deformations are not considered, the necessary computational power is considerably less than that required for deformable models, and useful information can often be extracted from relatively simple models that run quickly on low-cost computational hardware.

Rigid body models have been used in kinematics studies (i.e. to describe motion of the rigid segments, without consideration of the causes leading to movement) to assess the range of shoulder motions in rehabilitation and ergonomics applications (Johnson & Gill 1987; Engin & Tumer 1989; Klopcar et al. 2007). As an example of a model specifically tailored to address a clinical question, we implemented a rigid body model to investigate whether malpositioning of conventional shoulder implant components can cause impingement, leading to the notching observed in patients, finally inducing eccentric loosening and possible glenoid loosening (figure 2; Favre et al. 2008b). In an inverse dynamics approach, such models have been used to estimate joint moments in the whole upper limb during a specific motion (Barker et al. 1997).

**Figure 2.** (a) Notching of the humerus at the level of the inferior glenoid border in patients with a conventional shoulder implant and (b) rigid body model to investigate whether malpositioning of implant components can cause this notching through impingement, eventually leading to eccentric loading of the glenoid component and its loosening.
Most often, rigid body models have been used for rigid body dynamics, in combination with muscle force optimization techniques (described in detail in §2b later). Here, the rigid body models provide anatomical data, specifically the muscle moment arms and lines of action, as input to a coupled muscle force estimation method. Such models have been shown to predict accurately muscle moment arms of the rotator cuff in comparison with experimentally measured values (Gatti et al. 2007), supporting the use of rigid body models for calculation of moment arms, with the advantage that these can be easily computed for any position of the joint at any time, as opposed to those measured experimentally. In turn, the determined muscle forces may then be used to drive the rigid body kinematics in a forward dynamics approach. Here, the rigid body model serves for visualization of an induced motion, making muscle force estimation software more intuitive and facilitating user interaction with the model (Dickerson et al. 2007). Commercially available models for the whole musculoskeletal system (AnyBody Technology A/S, Aalborg, Denmark; SIMM, MusculoGraphics Inc., Santa Rosa, CA, USA) also incorporate muscle force optimization algorithms. These packages have been customized and used in several shoulder studies (Holzbaur et al. 2005; Langenderfer et al. 2005; Charlton & Johnson 2006).

While rigid body models are useful for many applications, they do have limitations. Most published rigid body models of the shoulder are limited by a simplified representation of the glenohumeral joint as an ideal joint, with predefined degrees of freedom. It has been approximated as consisting of three hinges with defined axes of rotation (Barker et al. 1997; Klopcar et al. 2007) or by defining it as an ideal ball-and-socket joint (van der Helm 1994b; Garner & Pandy 1999; Maurel & Thalmann 1999; Favre et al. 2008b). These simplifications prevent translations at the glenohumeral joint and thus limit studies on joint stability. Furthermore, the problem of ‘muscle wrapping’ requires some improvement. Accounting for physical contact between muscles and bones, or between muscles and other soft tissues, is a complicated issue that can limit accuracy in modelling muscle actions over large ranges of motions. This is a major problem as it directly affects the muscle moment arm and line of action (Charlton & Johnson 2001). It is sometimes solved artificially by defining so-called ‘via points’ through which the muscle is forced to pass or by replacing the complex bony geometry with simpler shapes (van der Helm et al. 1992; Garner & Pandy 2000; Holzbaur et al. 2005); but these techniques do not mirror the in vivo behaviour. More recent methods model the entire muscle volume using the FE method (Blemker et al. 2007). As a final limitation, rigid body models neglect tissue deformation and cannot be used to address some very important questions of shoulder biomechanics (such as arthroplasty, where quantifying mechanical bone stresses are important). However, these sacrifices in realism do yield a significant advantage in smaller requirements for computational power, allowing larger models of not only the shoulder but also often the entire upper limb or torso. This is essential in efficiently studying bi-articular muscles and the coupling between multiple joints.

(b) Muscle force estimation

Estimation of muscle loading is critical in predicting when tendon tears will occur. When tears have already been diagnosed, this information is required to
develop strategies for safely reconstructing them, or to optimize rehabilitation by focusing on the remaining viable muscles. It is also necessary to understand how the central nervous system controls the musculoskeletal system during specific tasks in order to best treat neurological or muscular deficiencies. Finally, accurately estimating the forces at the joint contact interface is fundamental to prosthesis design in preventing accelerated implant wear and premature failure.

In order to simulate how muscles are coordinated to move the arm or to hold it in a certain position, two parameters must be defined: first, an appropriate set of active muscles (muscle recruitment) and second, the distribution of force among these muscles to reach equilibrium. Early models of shoulder muscle force balance were two-dimensional systems that considered only a few muscles, and could be solved by simple analytical methods (Inman et al. 1944; De Luca & Forrest 1973; Poppen & Walker 1978; Bassett et al. 1990). While these models were limited to a simple arm movement (elevation) and included a restricted set of muscles, they nonetheless delivered important insights into some basic working principles of shoulder function. More importantly, they provided a technical foundation on which later three-dimensional models could be built to address more complex questions, necessitating the use of computers.

When comprehensively modelling the muscular forces at the shoulder, the main hurdle is of a mathematical nature. In the simplified case in which the glenohumeral joint is represented as a ball-and-socket joint (thus removing/constraining the three translational degrees of freedom), the system is governed by three equations describing the equilibrium in each rotational degree of freedom. The muscle forces are treated as unknowns in these equations. This system of three equations would have one unique solution only if no more than three unknowns were present. In actuality, the many muscles that cross the glenohumeral joint present a much less defined system. Muscles with large origins are often subdivided to allow for a differentiated action, as moment arm length and direction of tendon action can vary considerably within an individual muscle (van der Helm & Veenbaas 1991; Favre et al. 2005, 2009), so that many shoulder models regularly include more than 20 muscle segments. This yields a mathematically indeterminate system comprising more unknowns than equations and is characterized by an infinite number of possible solutions. The main issue is to find a method that systematically isolates a suitable solution among these infinite number of solutions.

Most computational methods tackle the indeterminacy issue using mathematical optimization. The forces are distributed among muscles in such a way that a chosen ‘cost’ function is minimized, while ensuring that these forces satisfy given physical constraints. The cost function can be based upon muscle stress, force, energy, fatigue, etc., and the constraints usually dictate that the muscle forces can apply tension only, must satisfy the equilibrium equations and fall within reasonable upper (tetanic muscle force) and lower (negligible force) muscle force limits (Karlsson & Peterson 1992). The first optimization models were developed to simulate muscular load sharing at other joints (Penrod et al. 1974; Seireg & Arvikar 1975), and the shoulder represents a more recent application. The first three-dimensional model of shoulder muscle force estimation was extensively described by Karlsson & Peterson (1992) and was later followed by the most frequently cited and implemented model to date (van der Helm 1994b).
One of the major problems in optimization techniques is the choice of an appropriate cost function. Comparisons with EMG activity have shown that some cost functions predict on–off muscle recruitment patterns better than others, but it is not yet clear what principles would dictate how muscles are recruited in vivo (Karlsson & Peterson 1992; van der Helm 1994a; Erdemir et al. 2007). Furthermore, muscle load sharing strategy is likely to differ between subjects, depending to some extent on the type of activity and varying in response to fatigue, mental demands and visual feedback or in the presence of musculoskeletal disorders, such as rotator cuff tears (Kronberg et al. 1991; Jensen et al. 2000; Steenbrink et al. 2006). Finally, co-contraction of antagonistic muscles can be predicted (Jinhaa et al. 2006), but it has been shown to confound conventional optimization-based models (Cholewicki et al. 1995; Dickerson et al. 2008).

In an attempt to overcome the drawbacks of analytical optimization techniques, experimentally based, EMG-driven models that were first developed for the lower back (McGill 1992) have been extended to the shoulder (Koike & Kawato 1995; Laursen et al. 1998; Langenderfer et al. 2005). In such models, the set of active muscles is identified in recordings of EMG activity for isolated shoulder positions. The muscle force is then estimated by assuming a linear relationship between EMG and force under isometric conditions. One advantage is that the recruitment of a particular muscle is directly indicated by the EMG measurements, and realistic muscle recruitment patterns can be immediately implemented in the model. In this way, co-contraction of antagonistic muscles may be directly accounted for and simulated. The main weakness of such models is that reliable EMG recordings of all relevant muscles must be available for the simulated position. This is technically demanding (even if possible) and brings with it the well-known difficulties inherent in EMG signal measurement and processing (De Luca 1997).

All muscle force estimation models are limited in their ability to be individualized, owing to the variability in anatomy and neuromuscular control, and this restricts the general applicability of a single model. Despite the limitations of these methods, and the difficulties in validating such models (to be discussed in §3b later), muscle force estimation models have been applied successfully to investigate a variety of clinical questions. They have been used to evaluate the influence of a prosthesis on the muscular forces (de Leest et al. 1996), to assess the influence of scapular neck malunion on shoulder function (Chadwick et al. 2004), to test tendon transfers (Magermans et al. 2004a,b) and to prevent overload injuries in wheelchair design and propulsion (van der Helm & Veeger 1996; Veeger et al. 2002; Lin et al. 2004; van Drongelen et al. 2005, 2006). Because muscle force estimation models must necessarily entail a muscle recruitment strategy, they give explicit insight into the manner in which the central nervous system drives the musculoskeletal system. Changes in the applied cost function or recruitment criteria directly affect the prediction of recruited muscles and can be varied to explore neuromuscular control hypotheses. The effect of a neurological or muscular deficiency can be assessed by scaling the allowed maximum relative force of selected muscles (van Drongelen et al. 2006). In a forward dynamics approach, muscle forces can be used to calculate joint torques and trajectory using the dynamics equations (Koike & Kawato 1995), and combined with rigid body models with the previously described advantage of motion visualization. Finally, such models are useful for investigating how joint stability is achieved, by considering
the intersection of the resultant force with the glenoid, with the joint remaining stable as long as the resulting joint force falls within the glenoid boundaries (van der Helm 1994b; Favre et al. 2005).

(i) A new paradigm for muscle force estimation

In an effort to avoid the previously described limitations that accompany traditional muscle force estimation methods (choice of an appropriate cost function, co-contraction prediction and requirements for EMG measurements), we have developed an algorithm to predict the muscle forces required for shoulder joint equilibrium. This algorithm implements a novel recruitment strategy that focuses on selecting muscles with a relative mechanical advantage, and a corresponding set of muscles that counterbalance secondary joint moments. Because the recruitment process is central to the new method, we describe it here briefly. A more comprehensive description of the entire algorithm can be found elsewhere (Favre et al. 2005).

In this muscle recruitment paradigm (figure 3), an external moment at the joint centre of rotation is decomposed into three orthogonal components. The Algorithm for Shoulder Force Estimation (ASFE) first recruits the muscles that
have the largest potential mechanical advantage in offsetting the greatest of the three external moment components, without any regard for the other two components (group 1). Here, potential mechanical advantage is defined by the muscle lever arms for the current position (Favre et al. 2009) multiplied by muscle cross section. In order to offset the two remaining components of the external moment, muscles that simultaneously oppose all three external components are recruited (group 2). Muscles that do not fit within these two groups are not active in the current loop (but may become active in later loops, thus allowing simulation of co-contraction, depending on which component of the remaining external moment becomes the greatest). The equilibrium force equations then attribute forces to the set of recruited muscles in proportion to each muscle’s cross-sectional area (thereby making the system mathematically determinate). The boundary conditions ensure that the assigned muscle forces are physiological (range in tension from zero to the tetanic muscle force) and the resultant muscle forces from this loop are then arbitrarily scaled down (typically by 95%) to ensure that the model converges and the external moment is not overshot. The whole process is iteratively repeated using the remaining external moment as input to the next loop, until all three components of the external moment are balanced. At the end, the resultant force is determined, and if the joint reaction force points outside of the glenoid (unstable joint), the simulation is restarted, but first giving all rotator cuff muscles a supplementary force.

This method has been shown to deliver realistic muscle recruitment patterns in comparison with EMG measurements (Favre et al. 2005). In order to validate the obtained joint reaction force, the performance of the ASFE and other optimization criteria, in comparison with the instrumented shoulder implant (Bergmann et al. 2007), is described in §2b(ii) below for a classic example.

(ii) Abduction in the scapular plane

Abduction was simulated with the ASFE at 0, 45, 90 and 120° with respect to the torso in the scapular plane. The arm weight (35 N) was applied at the middle of the arm (0.3 m from humeral head centre). Because the ASFE considers a fixed scapula, the rotation of the scapula was taken into account by rotating the external force vector according to a scapulohumeral rhythm ratio of 1 : 2.

Figure 4 shows the joint reaction force predicted by the ASFE and compares it with the reaction force reported from other studies (Poppen & Walker 1978; van der Helm 1994a; Terrier et al. 2008). Deviations in predicted joint resultant forces up to 90° can be explained by differences in model geometry (muscle segmentation, humeral head size, muscle size, muscle origin and insertion site) and recruitment strategy. The large deviation after 90° abduction is due to the ASFE incorporation of muscle co-contraction, which cannot be considered in the other models. Muscles of the rotator cuff and the deltoid, which represent the totality of muscles included by Poppen et al. and Terrier et al., also showed a decreased activity past 90° in the ASFE, except for the posterior deltoid segment. The rise in joint resultant force above 90° is due to other muscles. At 120° abduction, the majority of abductors externally rotate the humerus (table 2). Only the cranial segments of the subscapularis and pectoralis major can counterbalance external rotation, but they are also strong forward flexors. Here, other muscles such as teres major are activated to help balance these
components, even if such a muscle is a very strong adductor. Interestingly, in vivo measurements using instrumented shoulder prostheses (Bergmann et al. 2007) recently presented at the meeting of the European Society of Biomechanics have indicated that joint reaction forces increase as abduction exceeds 90° (Nikooyan et al. 2008). Although the ASFE is able to replicate this trend, it does not necessarily mean that the muscle forces found here correspond to an in vivo muscular contribution during abduction, as many physiologically plausible muscle force patterns can lead to a similar joint reaction force. Experimental measurements of muscular activity in postures above 90° of abduction are now required. However, it may indicate that co-contraction is a very important aspect of shoulder biomechanics, which has thus far been widely neglected.

(c) Deformable models

The FE method can simulate the deformations of complex systems that are otherwise difficult to assess and has been used to address a broad range of problems in the field of biomechanics and orthopaedics (Huiskes & Hollister 1993). FE modelling opens up a vast range of possibilities for simulating complex material phenomena such as nonlinear elastic and viscoelastic behaviours, plastic deformation, creep and fatigue failure behaviours.

Most FE models of the shoulder have been developed to specifically investigate glenoid fixation and loosening, generally relating excessive bone or cement stresses to failure. The influence of implant design parameters, such as peg or keeled glenoid anchorage (Lacroix et al. 2000), shape of implant components (Lacroix & Prendergast 1997; Buchler & Farron 2004; Terrier et al. 2006) or unconventional fixation type (Murphy & Prendergast 2005), has been studied using FE models. Finally, the FE method has been implemented in comparisons...
between cemented and uncemented prosthesis fixation (Gupta et al. 2004b,c), and testing the influence of cement thickness (Couteau et al. 2001; Terrier et al. 2005) or implant positioning on bone and cement stresses (Hopkins et al. 2004; Farron et al. 2006).

Table 2. Muscle segment moment arms at 120° abduction. (Abduction (+) or adduction (−) moment arms are given in the first column, forward (+) or backward (−) change in plane of elevation in the second, and internal (+) or external (−) axial rotation in the third column. The fourth column displays the forces attributed by the ASFE.)

<table>
<thead>
<tr>
<th>moment arm components</th>
<th>elevation (mm)</th>
<th>plane of elevation (mm)</th>
<th>axial rotation (mm)</th>
<th>force (N)</th>
</tr>
</thead>
<tbody>
<tr>
<td>anterior supraspinatus</td>
<td>17.19</td>
<td>14.21</td>
<td>−2.63</td>
<td>18.56</td>
</tr>
<tr>
<td>posterior supraspinatus</td>
<td>21.53</td>
<td>2.58</td>
<td>−2.63</td>
<td>18.56</td>
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<tr>
<td>cranial subscapularis</td>
<td>2.86</td>
<td>22.17</td>
<td>1.43</td>
<td>4.42</td>
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<td>−1.72</td>
<td>21.28</td>
<td>5.52</td>
<td>11.85</td>
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<td>−11.23</td>
<td>14.32</td>
<td>8.75</td>
<td>11.85</td>
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<td>cranial infraspinatus</td>
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<td>−4.20</td>
<td>10.61</td>
<td>18.28</td>
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<tr>
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<td>−11.63</td>
<td>18.28</td>
</tr>
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<td>−13.76</td>
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<td>18.28</td>
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<td>−15.76</td>
<td>−10.46</td>
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<td>−14.06</td>
<td>−14.32</td>
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<td>28.65</td>
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<td>5.17</td>
<td>0.00</td>
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<td>50.13</td>
<td>5.73</td>
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<td>caudal pectoralis major</td>
<td>−37.24</td>
<td>54.43</td>
<td>11.46</td>
<td>12.11</td>
</tr>
<tr>
<td>biceps caput longum</td>
<td>2.91</td>
<td>17.19</td>
<td>−10.02</td>
<td>22.13</td>
</tr>
<tr>
<td>biceps caput breve</td>
<td>2.91</td>
<td>31.51</td>
<td>0.00</td>
<td>30.63</td>
</tr>
</tbody>
</table>

Between cemented and uncemented prosthesis fixation (Gupta et al. 2004b,c), and testing the influence of cement thickness (Couteau et al. 2001; Terrier et al. 2005) or implant positioning on bone and cement stresses (Hopkins et al. 2004; Farron et al. 2006).

Sholder FE studies addressing other clinical shoulder questions are fewer. Interesting two-dimensional studies have considered the stress pattern in the supraspinatus tendon, trying to understand the mechanical origin of tears (Luo et al. 1998; Wakabayashi et al. 2003; Sano et al. 2006). Another study tried to quantify the influence of the shape of the humeral head on the stress distribution in the scapula with the intent to compare a normal with an osteoarthritic shoulder (Buchler et al. 2002). Finally, relative kinematics of implant components have been simulated using the FE method to study implant intrinsic stability (Hopkins et al. 2006, 2007).
The main limitations of deformable models usually lie in the definitions of boundary conditions and material properties that are employed. Measuring and describing the material properties of biological tissues is not at all simple, and most models necessarily implement idealized material properties. With regard to boundary conditions, \textit{in vivo} forces have been simulated by applying the joint resultant force only (Stone \textit{et al.} 1999; Couteau \textit{et al.} 2001; Andreykiv \textit{et al.} 2005). In more elaborate FE models (Lacroix \textit{et al.} 2000; Gupta \textit{et al.} 2004\textit{b,c}; Hopkins \textit{et al.} 2005, 2007; Murphy & Prendergast 2005), individual muscle contributions were assigned according to van der Helm (1994\textit{b}). Axial rotation of the humerus has been simulated by applying a gradually imposed displacement at a chosen muscle insertion and by restricting unwanted motions through non-physiological boundary constraints at the distal extremity of the humerus (Buchler \textit{et al.} 2002). In a later extension of the same model, this artificial boundary condition was removed, but the model was restricted to a two-dimensional representation and to the deltoid and rotator cuff muscles (Terrier \textit{et al.} 2008). Finally, investigating glenoid loosening requires a profound understanding of the failure mechanisms. FE models can predict mechanical factors such as bone-implant micromotion, wear or excessive stress, but the induced biological response is extremely complex and remains not yet fully understood.

Despite these limitations, results obtained from deformable models can still be directly transferred to clinical practice by defining the relative influence of surgically adaptable parameters (choice of implant, components positioning, use of cement, etc.) on the investigated consequence (stress shielding, aseptic loosening, etc.).

3. Model validation

To efficiently address scientific and clinical questions through a modelling approach, the goal is not to build a perfectly realistic model, but to create a sufficiently accurate representation of the aspect to be investigated. The complexity of a biological system, such as the shoulder, is such that some simplifications must be made in the modelling process, although each assumption introduces a potential source of error. To ensure that the imposed simplifications do not diminish the veracity of the simulation, validation is essential. The validation process confronts simulation results with reality, or, when this is not directly possible, with controlled experiments that approximate reality. Simulation results are compared against measurable parameters with the aim to identify inappropriate assumptions or simplifications that can then be adjusted to improve the fidelity of the model.

\textbf{(a) Validating rigid body models}

Simulated rigid body motion can be compared with experimentally measured kinematic data. For instance, the simulated reachable workspace of the arm can be validated against actual measurements of range of motions (Klopcar \textit{et al.} 2007). Rigid body models used for the quantification of moment arms can also be directly compared with \textit{in vivo} or \textit{in vitro} measurements (Garner & Pandy 2001; Gatti \textit{et al.} 2007). Finally, when combined with muscle force estimation, \textit{in vivo} measurements of maximum isometric muscle torques exerted at the joint and/or
the resultant kinematics can be used for comparison, although these only validate the global simulation quality and do not yield specific information on individual muscle forces (Garner & Pandy 2001).

\(b\) Validating muscle force estimation models

In an indeterminate system of equations, it falls on the modeller to restrict the number of considered solutions to those that can realistically occur \textit{in vivo}. As described above, muscle force estimation models deliver two main pieces of information: the \textit{set of recruited muscles} and the \textit{force} that these exert. EMG signals can be used to compare the timings of the muscle activities (Happee & van der Helm 1995) and to verify that the model activates a reasonable set of muscles (Karlsson & Peterson 1992; Happee 1994; van der Helm 1994b; Happee & van der Helm 1995; Nieminen \textit{et al}. 1995; Niemi \textit{et al}. 1996; Favre \textit{et al}. 2005), or they could also allow comparison of paralysis experiments (either pathological or neurotoxin induced) against model behaviour when specific muscles are removed from consideration. On the other hand, we are currently limited in our ability to quantify individual muscle force magnitude since no \textit{in vivo} muscular force measurement devices are currently available (Erdemir \textit{et al}. 2007), and EMG amplitude is a poor measure for validating the forces obtained by musculo-skeletal models (Inman \textit{et al}. 1952; van der Helm 1994b). Given the lack of reliable muscle force measurement techniques, results have generally been compared with those obtained with previous models. However, this approach cannot be considered a valid muscle force validation, but merely serves as an indication that two models represent reality in a similar way. Since this approach cannot root out problems with widely held assumptions, there is obviously a pressing need for better techniques to quantify \textit{in vivo} muscle forces.

\(c\) Validating deformable models

In the most straightforward validations of FE models, modelling results (surface strain patterns) have been directly compared with experiments performed under similar loading conditions, using an \textit{in vitro} strain gauge measurement (Couteau \textit{et al}. 2001; Gupta \textit{et al}. 2004a; Maurel \textit{et al}. 2005) or photoelastic techniques (Murphy & Prendergast 2005). As an example of clinical validation, bone formation around a retrieved specimen confirmed that the bone stress predicted by the model (disregarding other important factors) was within acceptable values (Ahir \textit{et al}. 2004). For a proper validation of an FE model, strict guidelines and ‘best practices’ have been suggested (Viceconti \textit{et al}. 2005). Unfortunately, the validation step is very often neglected in deformable models.

\(d\) Emerging technologies for model validation

In the past, validation often compared model results with experiments performed on cadavers. Emerging technologies now allow direct comparison with selected \textit{in vivo} measurements, bringing the models to a higher level of accuracy. Their use for validation of shoulder models is nascent (Dubowsky \textit{et al}. 2008; Terrier \textit{et al}. 2008), but is destined to increase. Rapid progress in the field of medical imaging opens new possibilities to measure rotation and translation of the glenohumeral joint during \textit{in vivo} movements using standard fluoroscopic...
sequences (Pfirrmann et al. 2002), open magnetic resonance imaging (MRI: Graichen et al. 2000) and biplanar X-rays (Bey et al. 2008). These quantities provide useful global criteria for a partial assessment of model performance of rigid body or contact models. Validation of the forces predicted by numerical musculoskeletal models of the shoulder has now been improved with direct measurements of glenohumeral contact forces using an instrumented implant (Bergmann et al. 2007) as well as enhanced techniques to measure in vivo muscle activity (Praagman et al. 2003, 2006; de Groot et al. 2004).

4. Outlook in numerical shoulder modelling

Implementation of more realistic modelling approaches to investigate stabilization of the glenohumeral joint is imperative (Veeger & van der Helm 2007). Since translations may no longer be small in comparison with rotations in the unstable shoulder, modellers may have to deviate from the simplification of the shoulder joint as a perfect ball-and-socket (Hopkins et al. 2006). If a priori (artificial) restrictions on translations are to be avoided, muscle force estimation models can play a valuable role in introducing muscle-driven stabilization of the joint.

Owing to the great individual variability in anatomy, patient-specific models may be needed to study specific skeletal deformities, and altered bone and soft tissue material properties, or for individual diagnosis and surgical planning. With semi-automatic extraction of anatomy from computed tomography and MRI images, models of individual patients are now plausible (Young et al. 2008). For studies on loosening of the glenoid component in shoulder arthroplasty, a more realistic representation of the underlying bone micro-architecture may improve the representation of the interface mechanics and force transmission in the bone, enhancing failure risk prediction (Ulrich et al. 1997; Pistoia et al. 2002). Also, long-term predictions of implant fixation could be improved by including bone mechanical adaptation laws into FE models (Beaupré et al. 1990; Cowin et al. 1992; Prendergast & Taylor 1994; Huijsses et al. 2000). Such FE models for the shoulder do exist but have been limited to two-dimensional analyses of the glenoid (Andreykiv et al. 2005; Sharma et al. 2007). Simulation of fibrous tissue interposition between the implant and bone could also be added (Weinans et al. 1990).

In this paper, shoulder models were treated as belonging to three main groups. Although these categories sometimes overlap already, as seen with the coupling of rigid body and muscle force estimation models, an integrated modelling approach can combine the advantages of the different models, offering new possibilities. For example, when studying the influence of implant component positioning (table 1), the integrated modelling approach would provide a tool to address simultaneously the interconnected implications in range of motions and anatomy (which could be investigated with a rigid body model), the changes in muscle activity and contact forces (which is studied with muscle force estimation models) and the deformations of the implant interface and implant fixation (information typically delivered by an FE model). In an effort to reduce computational expense, FE models rarely represent the shoulder as a whole. When possible, parts of the system are simplified (or neglected) and substituted with approximate boundary conditions. However, this can lead to erroneous
conclusions (Gupta & van der Helm 2004; Hopkins et al. 2005). For FE, in general, the benefits of relying on fully balanced external load regimes have been demonstrated (Duda et al. 1998; Speirs et al. 2007). Explicit incorporation of tissue deformations and failure further allow investigations into how these factors can affect segment motions and muscle force activity. Thus, through an integrated modelling approach, more realistic conditions can be implemented, yielding more reliable results. To this end, we see the FE method as the most promising framework. Modern commercial FE software packages allow simulation of large motions, and can implement the simplifying aspects of rigid body assumptions in a hybrid fashion, permit simultaneous inclusion of muscle force estimation and recruitment strategies, and allow determination of component deformations in critical locations. To this end, we are currently developing a model that combines the ASFE with an anatomically precise FE model of the glenohumeral joint (figure 5).

**Figure 5.** Integrated modelling approach combining the ASFE with an anatomically precise FE model of the glenohumeral joint: (a) FE (rigid body), (b) ASFE and (c) FE (deformable). Here, only a few muscle segments are represented on the three-dimensional model of the shoulder. The deformable muscles can wrap on the bones, relying on detection of contact in the FE software. The moment arms and lines of action of the muscles are computed in this position and sent to the ASFE. The muscle forces are returned as boundary conditions to the FE model. The infinitesimal motion of the arm is simulated within the FE model and the positional error between the obtained and the target positions is determined. This loop is reiterated until the positional error is less than a predefined value. Results obtained with this model will be validated against EMG patterns, glenohumeral contact forces for given activities, and clinical cases of muscle insufficiency.
In conclusion, numerical models of the shoulder have proven to be useful in a wide range of clinical applications. In the future, given our growing understanding of shoulder mechanics, advances in modelling methods and increases in computer power, numerical models should enable researchers to address ever more complex clinical questions and ultimately improve patient care.

References


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