

Towards Predictive Optimal Control of Detailed Closed-Loop Shoulder Models

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1. Introduction

Predictive optimal control simulations aim at anticipating the biomechanical consequences of clinical interventions and assistive devices. Unlike inverse dynamics, which relies on prescribed motion trajectories, predictive simulations generate movement by optimizing a performance criterion, such as the metabolic cost. This permits the determination of joint kinematics and muscle activations without requiring experimental measurements, offering a way to evaluate scenarios before they are physically implemented. These simulations are particularly valuable for shoulder applications. For instance, they can anticipate post-operative adaptations following tendon transfers or Reverse Total Shoulder Arthroplasty (RTSA). Another area where these simulations are useful is the design of assistive shoulder exoskeletons, as they allow researchers to predict kinematics and muscle excitations and tune the controller before expensive prototyping.

Despite this potential, widespread adoption has been hindered by high computational costs and numerical convergence challenges (Denton and Umberger 2023). To simplify the problem, existing studies that use predictive simulations often rely on models that simplify the shoulder girdle by coupling scapular motion to humeral angles via regression equations (Hamad et al. 2024). These models enforce a predefined shoulder rhythm, which prevents them from predicting novel kinematics when the system deviates from average physiological patterns, and they cannot accurately capture the specific contributions of thoracoscapular muscles (Seth et al. 2019). While detailed models with closed-loop kinematics

demonstrate high accuracy in inverse analysis, they have, to our knowledge, not been used for predictive optimal control because standard recursive solvers struggle with the differential-algebraic equations (DAEs) inherent in closed kinematic chains (Green et al. 2022). This work presents a framework that enables predictive simulations using a fully closed-loop kinematic shoulder model.

2. Methods

The predictive optimal control framework is implemented within the Odin software, which is well-suited for constrained mechanical systems. The software utilizes a Lie group geometric formalism in which each joint induces some constraints on the configuration variables. We employ a shooting-based optimal control scheme where the system equations in DAE form are solved using an implicit integration scheme. To ensure high computational efficiency, sensitivities for each system element are determined analytically, and gradients are computed via a discrete adjoint method within the integrator. This formulation provides exact gradients and robust convergence.

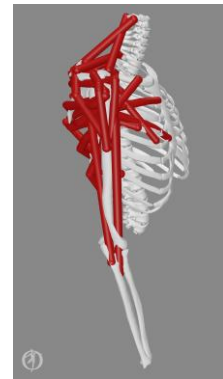


Figure 1. Musculoskeletal model of the shoulder incorporating a closed kinematic loop, adapted from Seth et al. (2019). Image rendered in OpenSim.

The musculoskeletal model is adapted from Seth et al. (2019) (Fig. 1). The model represents the shoulder girdle through a series of interconnected joints:

- Sternoclavicular joint: modeled as a universal joint.
- Acromioclavicular and glenohumeral joints: both modeled as spherical joints.
- Scapulothoracic joint: this joint closes the kinematic loop by constraining a point on the scapula to glide over the surface of the thorax, represented as an ellipsoid, and two more rotations.

The system is actuated by 33 Hill-type muscles, for which wrapping surfaces have been neglected for now. By resolving the closed-loop constraints through this numerical framework, the model avoids the need for predefined regression equations. This allows the scapula to move freely and the rhythm to be determined solely by the optimization of the chosen performance criterion.

3. Results and discussion

To evaluate the predictive capacity of the framework, we simulate two functional tasks. First, we simulate shoulder flexion by prescribing the initial pose and final glenohumeral elevation. The optimizer generates the muscle activations and kinematics that minimize an objective function comprising metabolic cost. The goal is to demonstrate the emergence of a shoulder rhythm and verify that the resulting motion is physiological for the given performance criterion. Second, we simulate shoulder shrugging by constraining the final clavicle elevation. This task highlights the framework's primary advantage compared to regression-based models: its ability to reproduce independent scapular control. Preliminary observations suggest the framework achieves performance comparable to state-of-the-art solvers for open-loop systems. Furthermore, initial results indicate that the inclusion of the closed-loop kinematic chain does not seem to lead to a substantial increase in computation time.

4. Conclusions

This study demonstrates the feasibility of simulating the shoulder girdle with detailed, closed-loop kinematics within a predictive framework. The primary contribution is establishing the computational viability of this numerical approach for systems characterized by complex topologies. While further model refinements such as muscle wrapping, subject-specific tuning and experimental validation might be required for clinical application, the ability to handle such topological complexity is a critical step toward advanced biomechanical tools. This framework paves the way for future work in pre-operative planning and the design of assistive exoskeletons, where a predictive understanding of the shoulder girdle is essential.

Conflict of Interest Statement

None

Contributor Roles

BM: Conceptualization, Methodology, Software, Investigation, Visualization, Writing – original draft;

VS: Methodology, Software, Validation; CS: Conceptualization, Writing - review & editing; OB: Conceptualization, Methodology, Supervision, Funding acquisition, Project administration, Writing - review & editing.

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Data, software, code availability

Odin: <https://doi.org/10.5281/zenodo.7468114>

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