Bioptim, a Python interface for Musculoskeletal Optimal Control in Biomechanics

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Abstract— **The abstract**
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I. INTRODUCTION

Many approaches coexist to discretize and solve optimal control problems (OCPs). In sports biomechanics, joint angle-driven algorithms are XXXX in which the joint angle time histories are xxx by series of quintic polynomial functions [REF Yeadon, Begon] or quartic splines [REF Leboeuf, Huchez]. Whereas evolutionary algorithms

The number of papers about optimal control or dynamic optimisation is growing in robotics and biomechanics (Fig. X), probably because of increasing computer power but also the emergence of advanced open source (and proprietary) librairies for algorithmic differentiation and NLP solvers. Tools dedicated to OCP in biomechanics are rare. As shown by the recently launched MOCCO, four interrelated components are required: i) musculoskeletal modeling software (multibody kinematics and dynamics, muscle dynamics, etc.), ii) a method for automatic differentiation, iii) a discretization approach, and iv) a nonlinear programming (NLP) solver. Generic optimal control software (e.g. GPOPS-II [ref], Muscod-II [ref], Acado [ref]) provides solutions for component ii to iv but xxx. Since biomechanics is a community of software users [REFS], we believe that dedicated optimal control software will request a graphic user interface or at least a complete interface with a open source high-level language (e.g. Python) with a low-level core (C++) for efficiency.

When developing such software, we should consider that human movements are often multiphase (i.e. with different dynamics due to change in contact forces), [trouver d'autres], and models should be personalized, which may require several trials and some parameters' identification. Moreover, in contrast to the inverse flow which relies on measures, solving the ordinary differential equations (ODEs) of motion may result in unanticipated behaviours , ranging from non-physiological states to singularities. Either convenient constraints' definition and XXXXX,

Lifting and relaxing OCPs, DMS et DC Constraints vs cost

While CasADi is used in MOCCO mainly for its interface to ipopt (ADOL-C being used for automatic differentiation), this tool was first and foremost designed for algorithmic differentiation and is consequently widely used for NLP to reduce the cost and increase the accuracy of gradient

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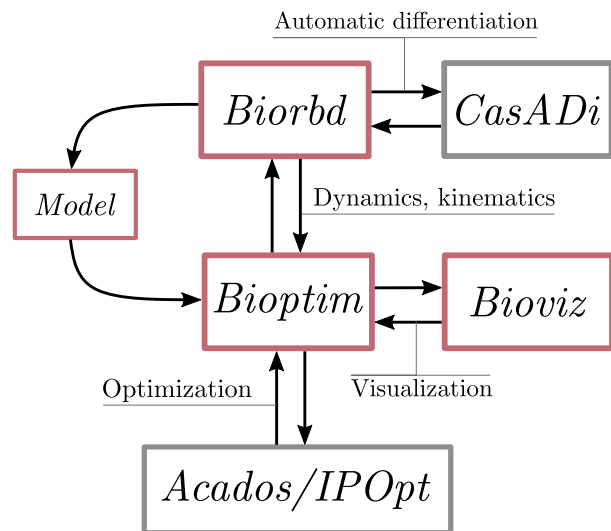[*] author#1@umontreal.ca

Fig. 1: *Bioptim* dependencies flowchart. The red-boxed software are developed by the S2M team.

and Hessian compared to finite-difference method. Acados, a recent NLP solver dedicated to DMS, was recently launched by the same research group as CasADi taking advantage of the algorithmic differentiation for real-time applications. Some applications, such as the real-time estimation of muscle forces, presently solved by inverse approach [REF] (from inverse dynamics to static optimization) or hybrid approach like the EMG-assisted algorithm in CEINMS [REF], become possible [citer article François-Amedeo]

The objective of the present paper is to introduce an innovative optimal control software for OCPs in biomechanics with the following features: Written in Python with Real-time capability

The paper is organized as follow:

II. IMPLEMENTATION AND DESIGN

A. Implementation and dependencies

Bioptim is the top layer of a succession of software on which it depends to perform various calculations (*Biorbd*: dynamics; *CasADi*: automatic differentiation; *IPOpt, Acados*: optimization; *Bioviz*: visualization). Within this software bundle, Bioptim's main role is to shape the problem in order to allow its dependencies to communicate efficiently, while providing an intuitive and flexible interface to the user (Fig. 1). Therefore, it was chosen to be written in Python for its flexibility and its widespread use among researchers. However, all intensive calculations behind the interface are performed in C or C++, keeping *Bioptim* both fast and easy to customize.

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B. Design

Bioptim shapes and solves optimal control problems whose two required entries are a model (*.bioMod* file) and an OCP. The model file contains the geometrical characteristics, the mass and inertia parameters, the geometrical markers and possibly the muscular information of the model. It also allows the user to design or import meshes for visualization purposes. The OCP is implemented as a succession of nonlinear problems (NLPs) for allowing the formulation of multi-stage OCPs. Each NLP has the following attributes: a dynamics type, a list of objective function, constraints, initial guesses, a number of shooting points and the duration of the problem. Based on these inputs, *Bioptim* properly sets up the multiple shooting transcription of the OCP, with appropriate continuity constraints in the case of multiple NLPs, and shapes it up to feed the chosen non-linear solver (Ipopt or Acados).

1) Dynamics types: The dynamics type defines which variables are states ($\mathbf{x}$), which ones are controls ($\mathbf{u}$) and which ones are parameters ($\mathbf{p}$). Then, it implements the ordinary differential equation governing the state transition:

$$\dot{\mathbf{x}} = f(\mathbf{x}, \mathbf{u}, \mathbf{p}). \tag{1}$$

More than ten dynamics are implemented in *Bioptim*, among which the controls can be muscle excitations/muscle activations/joint torques, the states can be joint kinematics/muscle activations, including/excluding contacts, etc. Even if these dynamics types exhaustively span the current usages in biomechanics, a custom dynamics type is also pre-implemented to allow easy problem customization.

2) Objective functions: Accordingly to the optimal control formalism, there are two main types of objective functions, namely Lagrange and Mayer. Lagrange types are running objectives, integrated over the whole NLP. Mayer types are time-specific objectives. Classically, they correspond to a terminal objective, but to be more versatile, they can be defined at any instant in *Bioptim*.

These objective functions can depend on any of the optimization variable, *i.e.* the controls, the states, the parameters and the duration of the problem. A lot of objective function types are already implemented in *Bioptim* ($>$ 20), among which tracking/minimizing, on the states/controls/geometrical markers/contact forces/problem duration, etc. Should one go missing, a custom objective type is also pre-implemented.

When declaring the desired list of objective function for a given NLP, each objective function type is associated with a weight, and the user can flexibly choose on which components of the vector variables the objective must apply. If applicable (for tracking objective functions mainly), the user must also specify the numerical target of the objective.

3) Constraints:

III. EXAMPLES

In the following, seven applications are presented to illustrate the versatility of Bioptim and to give a practical overview on how to use its main features. The performances and the Github links of each OCP are summarized in Tab. II.

A. Muscle activation driven pointing task

The goal was to achieve a muscle activation driven pointing task using a 2-DoF, 6-muscle arm model. In addition to muscle-induced torques, pure torques could compensate for the model weaknesses.

Term #1 of the objective function (Tab. I) corresponds to the pointing tasks described by a Mayer term (heaviest weight), to superimpose two markers, the first one fixed in the ulna system of coordinates and the second one fixed in the scene. Terms #2 and #3 were added for control regularization (muscle activation and torques) and #4 for state regularization. The movement lasted for 2 seconds and was discretized using 51 shooting nodes.

TABLE I: Objective terms of the activation-driven pointing task. The names of the functions correspond to the nomenclature used in *Bioptim*.

	Type	Function	Weight
#1	Mayer	ALIGN_ MARKERS	$1e6$
#2	Lagrange	MINIMIZE_ MUSCLE_ CONTROL	$1e1$
#3	Lagrange	MINIMIZE_ TORQUE	$1e1$
#4	Lagrange	MINIMIZE_ STATE	$1e1$

The problem was solved using IPOPT and ACADOS resulting in two significantly different solutions. ACADOS provided a 16 times smaller optimized cost (Tab. II), which illustrate the pitfalls of local minima as well as the benefits of having straightforward access to different solvers. Indeed, the ACADOS-based solution (Fig. 2, top) makes good use of gravity to minimize the control inputs, while the IPOPT-based solution (Fig. 2, bottom) moved the arm in the opposite direction and was stuck in a local minimum (still achieving the task though). It is worth mentioning that for the purpose of this illustration, no constraint was given about the shoulder range of motion to ensure physiological muscle trajectories.

B. Quaternion base twisting somersault

The goal was to maximize the twist rotation (ϕ) in a backward somersault. The model is composed of a 6-DoF root segment and two 1-DoF torque actuated arms. The OCP was solved for two models. First, rotations of the root segment were expressed as Euler angles. They were expressed as a quaternion for the second model. The objective functions were written as follow:

$$\mathcal{J} = - \underbrace{\int_0^T \dot{\phi} dt}_{MINIMIZE\_TWIST} + 1 \times 10^{-6} \underbrace{\sum_{i=1}^{2} \int_0^T \tau_i^2 dt}_{MINIMIZE\_TORQUE} \quad , \quad (2)$$

where T in the duration of the movement and τ_i is the torque control of the ith arm DoF. The first term of the objective

function (Eq. 2) corresponds to maximizing the twist velocity and the second term is for control regularization.

The movement lasted for approximately 1 second and was discretized in 100 shooting nodes. The solutions for both models were similar (Fig. **??**) highlighting the equivalence of the two rotation representations. Euler angles have the advantage to be easily interpretable, but they suffer from the loss of a DoF at the gimbal lock. The use of quaternion representation is advantageous for numerical stability when a joint is free to rotate on a wide three-dimensional range for motion.

C. Multiphase torque driven walking cycle

The goal was to estimate joint torques which are dynamically consistent during one gait cycle from the first heel strike to the end of the swing phase using a 3D one-leg torque driven model with 12 DoFs.

The experimental joint angles (obtained from markers using an extended Kalman filter), ground reaction forces and moments were tracked:

$$\mathcal{J} = \sum_{i=1}^{N_i} \left(\underbrace{1 \times 10^5 (\|q_p - q_m\|^2)}_{TRACK\_STATE} \right. \tag{3}$$

$$+ 1 \times 10^{-2} (\underbrace{\| \sum_{c=1}^{N_c} F_c - F_m \|^2}_{TRACK\_FORCES}) \tag{4}$$

$$\left. + 1 \times 10^{-2} (\underbrace{\| \sum_{c=1}^{N_c} OC \wedge F_c - M_{m,O}\|^2}_{TRACK\_MOMENTS}) \right) \tag{5}$$

Where N_i and N_c are the number of time frames and contact point, respectively. The tracking consisted of the minimization between predicted q_p and calculated q_m joint trajectories (first term - Eq. 3) and between the sum of contact force and moments for each contact point F_c and measured forces and moments F_m, M_m (second and third term - Eq. 3 and Eq. 5).

The interaction between the ground and the foot was modelled using a 4-contact point model located at the heel and the forefoot (first and fifth metatarsi and toes - digit of the second toe). The stance phase was divided in three to follow the natural rolling movement of the foot from heel strike to toe off: heel, flatfoot and forefoot contacts. A constraint of non-slipping (NON_SLIPPING) and unilateral contact force (CONTACT_FORCE) were added for each stance phase. The use of the IMPACT state transition allowed to represent the gain of contact from a system without any contact (swing phase) to a system with contacts (heel strike) [ref thesis Felis - articles?].

Based on force plateform data and markers position, each phase had a definite time inducing a complete simulation time
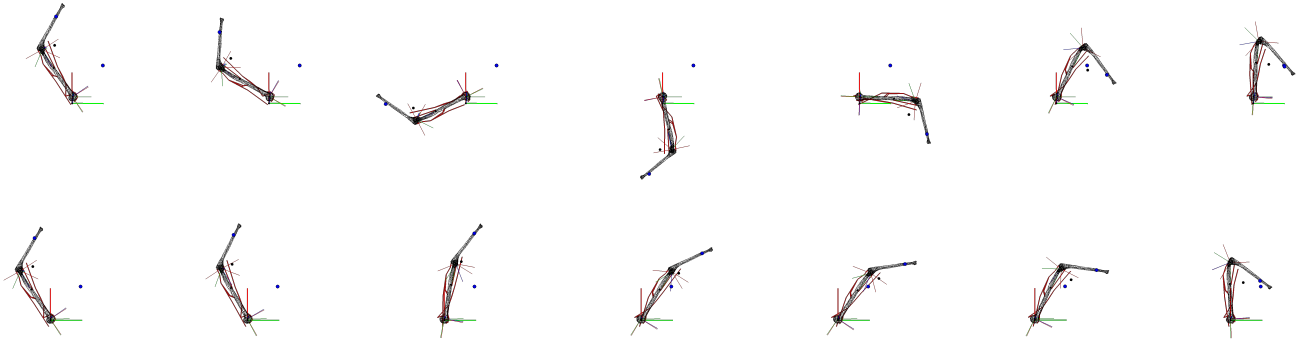
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Fig. 2: Snapshots of an optimized muscle activation driven pointing task. Top: using ACADOS. Bottom: using IPOPT.
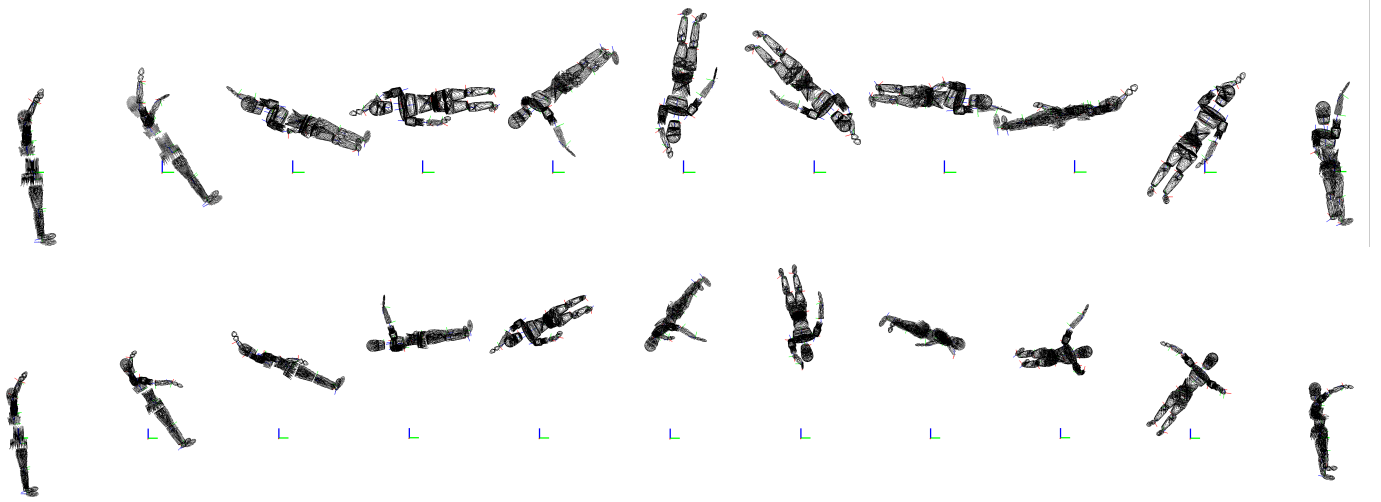

Fig. 3: Snapshots of a maximally twisting somersault driven by torque actuation. Top: Euler angles. Bottom: quaternion.

of 0.93 s and was discretized in 94 intervals. The solution was able to reproduce a complete gait cycle [value RMSE - better with 3 contact points?] (Fig. 4).
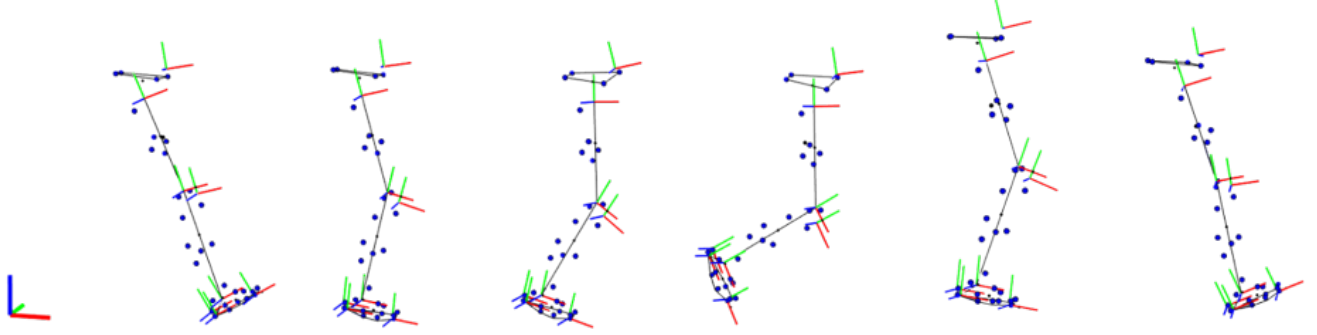
Fig. 4: Snapshots of a walking gait cycle driven by torque actuation.

TABLE II: Overview of computational results for the different OCPs cases and links to detailed implementations. * stands for free time OCP, otherwise it is fixed.

		Activation-driven pointing		Ex# 2		Ex# 3	
Setup	# states $\boldsymbol{x}(t)$	2		–	–	–	–
	# control $\boldsymbol{u}(t)$	8		–	–	–	–
	# shooting nodes	51		–	–	–	–
	OCP duration (s)	2		–	–	–	–
		IPOpt	ACADOS	IPOpt	ACADOS	IPOpt	ACADOS
Solve	# NLP iterations	27	21	–	–	–	–
	Optimized cost	6959.3	427.5	–	–	–	–
	Time to convergence (s)	9.9	0.19	–	–	–	–

IV. Discussion

The objective of *Bioptim* is to solve a variety of biomechanical OCPs with minimal programming with high performance in terms of computational time and cost value. The main observation of the summary Table X of the six examples are: i) the ability to use torque-drive to excitation-driven models (and their combination) and dynamics with/without contact ii) a combination of cost functions and constraints iii) solve advanced OCPs in a few seconds or minutes, that were previously known to take hours. iv) easily switch from one NLP solver to another.

Through various examples, we highlighted key features of bioptim including

A. *Utiliser des solveurs spécifiques et open source à DMS (Acados)*

Bioptim takes advantage of several open source libraries to achieve a robust and/or fast convergence, especially CasADi combined with NLP solver namely ipopt or Acados, respectively. Whereas the choice of ipopt or Acados requires limited effort for the user, basic knowledge of both NLP solvers may help to determine appropriate weightings and best options. By comparison to previous studies, OCPs were solved much faster (e.g. XXXX s in [Colombe] vs XX s here;)

B. *Différenciation algorithmique (ADOL-C dans Moco pour les collocations) ... MX vs SX*

C. *DMS (privilégié dans biorbdoptim) vs direct collocation (link)*

While the debate remains about the performance of direct collocations versus DMS, the development of bioptim was mainly oriented toward DMS, especially for the parallel computing. Nevertheless, existing collocations (Legendre) available in CasADi can be used and Acados proposes both explicit and implicit Runge-Kutta, the latter being a collocation approach. While implicit RK showed better convergence according to our own experience with Acados, explicit RK4 shows faster convergence in most of our implemented examples (those of the present paper and those available with biorbdoptim to present most of the features). In contrast to several papers [REFS], DMS was not a limitation to the performance (cost value and time to convergence) in our OCPs and is used in the most advanced real-time XXXX (Acados)

D. *"Python based but fast" ... biomécanique communauté d'utilisateurs*

Since bioptim is written 100

Its performance is not affected by our Python architecture since the components of the OCP (i.e. continuity constraints which rely on the forward and muscle activation dynamics, paths constraints, Mayer and Lagrange costs) are all expressed as CasAdi trees for algorithmic differentiation and evaluation in C++ by the CasADi virtual machine.

Inspired by the real-time graphics from MUSCOD-II, biordbdoptim proposes a series of figures to analyze the solution at each iteration with minimal computational cost thanks to a XXX protocole. Other save and load options are valuable for post-processing analysis.

E. *Custom en python et pas en C++*

F. *Fast resolution = multistart*

Fast solvers offer the opportunity to use multistart on complex problems in order to circumvent the obstacle of local minima [1], [2] or to get meaningful initial solutions from simpler problems, for guiding the resolution of the sought problem.

G. *Multiphase*

H. *Cost vs constraints ... relâcher le problème simplement*

I. *Limitations*

Bioptim is already a mature solution for solving OCP in biomechanics, however some limitations should be raised. First, it is based on the musculoskeletal package developed in our laboratory, namely, biorbd. While the strength of biorbd is to be fast, XXX, and CasADi-friendly for the algorithmic differentiation of most of the kinematic and dynamic functions [REF], it is not as advanced as OpenSim or Anybody in terms of biomechanical features. The few examples (section X) highlighted simple to advanced models. Currently, biorbd does not include a model builder with a GUI. Some Opensim models can be translated to biorbd's models using Python's functions [LINK] but our MSK library does not support multiple wrapping objects, non-orthogonal DoFs between two bodies, compliant contact force models (e.g. [SmoothSphereHalfSpaceForce [52]]) or muscle-tendon equilibrium yet. As seen in Mocco and other MSK models for OCPs, wrapping objects are rare due to computational cost and required optimization when a line of action is in contact with more than one object. Via points [REF] and pre-processed moment arms (to be expressed as polynomial functions of crossed DoFs) are often preferred. In example X, the model differences (Opensim vs Biorbd), especially at the knee may explain the XXXX. Muscle-tendon equilibrium and model builder are already planned and the former will either required an additional optimisation procedure to achieve the equilibrium as in CEINMS [REF] or adding the length of muscle part with explicit constraints of XXXX in the OCP like in [REF]. Algorithms available in RBDL (core of biorbd for XXX) for ellipsoid foot model XXXXX (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6693511/).

A second limitation, which is to be adressed, is the fact that bioptim does not support multithreading in all conditions, e.g.: multiphase or multi-trial OCPs, Acados (despite its nfold faster convergence compared to Ipopt in multithread). Based on our experience about multithreading based on the architecture of bioptim (only the integration of the different shooting intervals are parallelized), the best advantage was found when the Hessian is calculated by algorithmic differentiation. Being the most costly part of the OCP, multithreading gives nearly linear reduction of the convergence time up to X threads. Such a gain is not found when the Hessian is updated using the BFGS quasi-Newton algorithm (i.e. the 'limited-memory' option in ipopt).

J. Future directions

Realtime estimation using MHE

MOOCP .. using front pareto

Prediction of adaptations due to muscular fatigue using NMPC

In line with the current studies of our research group, the future developments will first include nonlinear model predictive control and MHE (see example X) to predict optimal performances in repetitive tasks that generate muscular fatigue and real time estimation of joint torques and muscle forces, respectively. As shown in our previous studies [REFS] the analysis of a series near-optimal solutions is relevant in sport (but also in rehabilitation and ergonomics) and further efforts about multiobjective OCP of human performances are anticipated.

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APPENDIX

The appendix