Supplementary material of the journal paper:

Subject-exoskeleton contact model calibration leads to accurate interaction force predictions

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1) Description of the optimal control problem

Parameterization of states and controls

The direct collocation method consists of discretizing the states in several intervals (x^0, x^1, … x^N). These intervals are, in turn, discretized with some collocation points, for example x_1^0, x_2^0, x_3^0 for the interval between x^0 and x^1, x_1^1, x_2^1, x_3^1 for the interval between x^1 and x^2, and so on (see Fig. 1). All state points are design variables in the optimization problem. States are considered to be parameterized within each interval as Lagrange polynomials. The Lagrange parameterization has the following form:

$$L_j(\tau) = \prod_{r=0, r\neq j}^{3} \frac{\tau - \tau_r}{\tau_j - \tau_r} \quad (1)$$

where *r* are the collocation points, and *j* are the number of polynomials that define the polynomial basis (one for each point of the interval). Then, a state variable at time *t* can be approximated as a function of the state values at the collocation points of the time interval *i*. If the time discretization is regular (with time intervals of width *h*), the expression of the state becomes:

$$\tilde{x}^i(t) = \sum_{r=0}^{3} L_r\left(\frac{t - t_i}{h}\right) x_r^i \quad (2)$$

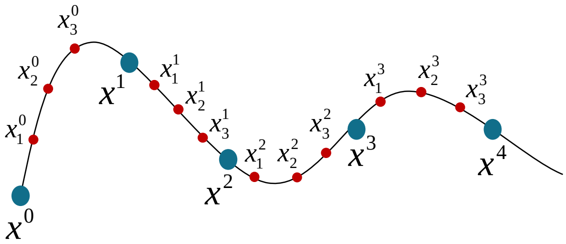

Figure S1. Discretization of states and parameterization with Lagrange polynomials

Controls are usually only optimized at the beginning of each time interval (u^0, u^1, … u^N), as in this study. However, to avoid having a constant control at each time interval, we can approximate them as Lagrange polynomials within each time interval as well. In this case, the polynomial bases consists of two polynomials, at the beginning and at the end of each time interval:

$$L_j^u(\tau) = \prod_{m=0, m\neq j}^{1} \frac{\tau - \tau_r}{\tau_j - \tau_r} \tag{3}$$

Then, the expression of the control values within a time interval is quite simple:

$$\tilde{u}^i(t) = \sum_{r=0}^{1} L_r^u\left(\frac{t-t_i}{h}\right) u_r^i = u_0^i \frac{t-t_f^i}{-h} + u_1^i \frac{t-t_0^i}{h} \tag{4}$$

Variables derived from states and controls

With the introduced state discretization, the derivative of the states becomes quite straightforward. If the time discretization is regular along all intervals, the expression of state derivative at time t_j^i (time j of time interval i) is:

$$\tilde{\dot{x}}^i(t_j^i) = \frac{1}{h}\sum_{r=0}^{3} \dot{L}_r(\tau_j) x_r^i \equiv \frac{1}{h}\sum_{r=0}^{3} C_{r,j} x_r^i \tag{5}$$

where C is a constant matrix for all time intervals.

In the optimization, we will need to impose continuity constraints, therefore we will need to impose a constraint between the last point of an interval and the first of the following one. With the introduced discretization, we can approximate the state at the last collocation point of an interval as a function of the states at collocation points as follows:

$$\tilde{x}_0^{i+1} = \sum_{r=0}^{3} L_r(1) x_r^i \equiv \sum_{r=0}^{d} D_r x_r^i \tag{6}$$

where D is a vector constant for all time intervals (as long as the time discretization is regular).

Integrals of variables parameterized with Lagrange polynomials also have simple expressions. For instance, the integral of a state becomes as follows:

$$\int_{t_k}^{t_{k+1}} \tilde{x}_k(t)\,dt = h\sum_{r=0}^{d}\int_{0}^{1} L_r(t)\,dt\,x_{k,r} := h\sum_{r=1}^{d} B_r x_{k,r} \qquad (7)$$

Where B is a vector constant for all time intervals (as long as the time discretization is regular). The linear dependence of state values, state derivative and integrals respect to state values at collocation points facilitates the direct collocation formulation.

Design variables

Phase A:

States (one value at each collocation point)	Coordinates: $q_{x\,foot}, q_{y\,foot}, q_{r\,foot}, q_{h\,ankle}, q_{h\,knee}, q_{h\,hip}, q_{e\,ankle}, q_{e\,knee}, q_{e\,hip}$ Velocities: $\dot{q}_{x\,foot}, \dot{q}_{y\,foot}, \dot{q}_{r\,foot}, \dot{q}_{h\,ankle}, \dot{q}_{h\,knee}, \dot{q}_{h\,hip}, \dot{q}_{e\,ankle}, \dot{q}_{e\,knee}, \dot{q}_{e\,hip}$ Accelerations: $\ddot{q}_{x\,foot}, \ddot{q}_{y\,foot}, \ddot{q}_{r\,foot}, \ddot{q}_{h\,ankle}, \ddot{q}_{h\,knee}, \ddot{q}_{h\,hip}, \ddot{q}_{e\,ankle}, \ddot{q}_{e\,knee}, \ddot{q}_{e\,hip}$
Controls (one value per mesh interval)	Jerks $u_{\dddot{q}_{x\,foot}}, u_{\dddot{q}_{y\,foot}}, u_{\dddot{q}_{r\,foot}}, u_{\dddot{q}_{h\,ankle}}, u_{\dddot{q}_{h\,knee}}, u_{\dddot{q}_{h\,hip}}, u_{\dddot{q}_{e\,ankle}}, u_{\dddot{q}_{e\,knee}}, u_{\dddot{q}_{e\,hip}}$ Joint torques $u_{T_{h\,ankle}}, u_{T_{h\,knee}}, u_{T_{h\,hip}}, u_{T_{e\,ankle}}, u_{T_{e\,knee}}, u_{T_{e\,hip}}$ Ground-reaction forces (in global frame) u_x^{GRF}, u_y^{GRF}
Parameters	Foot-ground contact parameters: Stiffness (*k*), damping (*c*), locations of the centre of the spheres with respect to the calcaneus frame ($x_{calcaneus}^{front\,sphere}$, $y_{calcaneus}^{front\,sphere}$, $x_{calcaneus}^{heel\,sphere}$, $y_{calcaneus}^{heel\,sphere}$)

where q , $\dot{q}$, $\ddot{q}$ and $\dddot{q}$ are the coordinates of the model and their derivatives (velocities, accelerations and jerks), respectively. *h* stands for human, *e* for exoskeleton, *T* for torque, and *GRF* for ground reaction force.

Phase B:

States (one value at each collocation point)	Coordinates: $q_{x\ foot}, q_{y\ foot}, q_{r\ foot}, q_{h\,ankle}, q_{h\,knee}, q_{h\,hip}, q_{e\,ankle}, q_{e\,knee}, q_{e\,hip}$ Velocities: $\dot{q}_{x\ foot}, \dot{q}_{y\ foot}, \dot{q}_{r\ foot}, \dot{q}_{h\,ankle}, \dot{q}_{h\,knee}, \dot{q}_{h\,hip}, \dot{q}_{e\,ankle}, \dot{q}_{e\,knee}, \dot{q}_{e\,hip}$ Accelerations: $\ddot{q}_{x\ foot}, \ddot{q}_{y\ foot}, \ddot{q}_{r\ foot}, \ddot{q}_{h\,ankle}, \ddot{q}_{h\,knee}, \ddot{q}_{h\,hip}, \ddot{q}_{e\,ankle}, \ddot{q}_{e\,knee}, \ddot{q}_{e\,hip}$
Controls (one value per mesh interval)	Jerks: $u_{\dddot{q}_{x\ foot}}, u_{\dddot{q}_{y\ foot}}, u_{\dddot{q}_{r\ foot}}, u_{\dddot{q}_{h\,ankle}}, u_{\dddot{q}_{h\,knee}}, u_{\dddot{q}_{h\,hip}}, u_{\dddot{q}_{e\,ankle}}, u_{\dddot{q}_{e\,knee}}, u_{\dddot{q}_{e\,hip}}$ Joint torques: $u_{T_{h\,ankle}}, u_{T_{h\,knee}}, u_{T_{h\,hip}}, u_{T_{e\,ankle}}, u_{T_{e\,knee}}, u_{T_{e\,hip}}$ Ground-reaction forces (in global frame): u_x^{GRF}, u_y^{GRF} Subject-exoskeleton contact forces (in local human body frame) $u_x^{SE\,C\ pelvis}, u_y^{SE\,C\ pelvis}, u_x^{SE\,C\ femur}, u_y^{SE\,C\ femur}, u_x^{SE\,C\,tibia}, u_y^{SE\,C\,tibia}$
Parameters	Subject-exoskeleton contact parameters: For each spring-damper system (at the pelvis, femur and tibia): Translational and rotational stiffness (*kx*, *ky*, *kr*) and location of the origin of the spring-damper in the corresponding human body ($x_{human\,body}^{origin}$, $y_{human\,body}^{origin}$).

where *SE C* stands for subject-exoskeleton contact force.

Phases C1 and C2:

States (one value at each collocation point)	Coordinates: $q_{x\ foot}, q_{y\ foot}, q_{r\ foot}, q_{h\,ankle}, q_{h\,knee}, q_{h\,hip}, q_{e\,ankle}, q_{e\,knee}, q_{e\,hip}$ Velocities: $\dot{q}_{x\ foot}, \dot{q}_{y\ foot}, \dot{q}_{r\ foot}, \dot{q}_{h\,ankle}, \dot{q}_{h\,knee}, \dot{q}_{h\,hip}, \dot{q}_{e\,ankle}, \dot{q}_{e\,knee}, \dot{q}_{e\,hip}$ Accelerations: $\ddot{q}_{x\ foot}, \ddot{q}_{y\ foot}, \ddot{q}_{r\ foot}, \ddot{q}_{h\,ankle}, \ddot{q}_{h\,knee}, \ddot{q}_{h\,hip}, \ddot{q}_{e\,ankle}, \ddot{q}_{e\,knee}, \ddot{q}_{e\,hip}$
Controls (one value per mesh interval)	Jerks: $u_{\dddot{q}_{x\ foot}}, u_{\dddot{q}_{y\ foot}}, u_{\dddot{q}_{r\ foot}}, u_{\dddot{q}_{h\,ankle}}, u_{\dddot{q}_{h\,knee}}, u_{\dddot{q}_{h\,hip}}, u_{\dddot{q}_{e\,ankle}}, u_{\dddot{q}_{e\,knee}}, u_{\dddot{q}_{e\,hip}}$ Joint torques: $u_{T_{h\,ankle}}, u_{T_{h\,knee}}, u_{T_{h\,hip}}, u_{T_{e\,ankle}}, u_{T_{e\,knee}}, u_{T_{e\,hip}}$ Ground-reaction forces (in global frame): u_x^{GRF}, u_y^{GRF} Subject-exoskeleton contact forces (in local human body frame) $u_x^{SE\,C\ pelvis}, u_y^{SE\,C\ pelvis}, u_x^{SE\,C\ femur}, u_y^{SE\,C\ femur}, u_x^{SE\,C\,tibia}, u_y^{SE\,C\,tibia}$
Parameters	-

Note that foot-ground and subject-exoskeleton contact forces can be calculated as a function of kinematics. However, we included them as controls to get a better convergence. During the optimization, those values can change and only at the optimal solution will be equal to the ones calculated as a function of kinematics.

Formulation of constraints

In all phases we included the following constraints:

- Continuity constraints. The state value at the end of each mesh interval must be the same as the first value of the following interval. Following Eq. (6):

$$\tilde{x}_0^{i+1} - x_0^{i+1} = 0 \tag{8}$$

- Dynamic constraints. The derivatives of the state variables at the intermediate collocation points of each mesh interval must be consistent with the approximated values calculated using the Lagrange polynomials (Eq. (5)):

$$\tilde{\dot{x}}^i \left(t_j^i\right) - \dot{x}\left(t_j^i\right) = 0 \tag{9}$$

- Path constraints. Since we used an implicit dynamic formulation, the equations of motion are included as constraints at the beginning of each mesh interval:

$$\left[\mathrm{M}(q)\right]\ddot{q} + C(q,\dot{q}) + G(q) - \tau_T - \tau_{GRF} - \tau_{SEC} = 0$$

  where M is the mass matrix of the multibody system, C is the vector of centrifugal terms, G is the vector containing the gravity terms and τ_T, τ_{GRF} and τ_{SEC} are the the vectors of generalized forces due to joint torques, GRF and subject-exoskeleton interaction, respectively.

Additionally, since we considered foot-ground and exoskeleton contact forces as controls, we included, at the beginning of each time interval, the constraints to impose that those controls are equal to the ones calculated as a function of kinematics:

$$\frac{GRF}{F_0} - u^{GRF} = 0 \tag{10}$$

$$\frac{F^{SEC}}{F_0} - u^{SEC} = 0 \tag{11}$$

where F_0 = 300 Nm was used to normalize GRF (ground reaction forces) and F^{SEC} (subject exoskeleton contact forces).

Cost function terms

The expression of the cost function contains minimization and tracking terms:

- Minimization terms:

Joint torques (Phase A)	$$J = w_{\min T} \sum_{i}^{nT} u_{T_i}^2 \qquad (12)$$
Jerks (All phases)	$$J = w_{\min \dddot{q}} \sum_{i}^{nDOF} u_{\dddot{q}_i}^2 \qquad (13)$$
Subject-exoskeleton (Phase B – only components with no experimental information, Phase C – all components)	$$E_c = \int \left[F_x(t)\dot{x}(t)\right]^2 dt + \int \left[F_y(t)\dot{y}(t)\right]^2 dt + \int \left[M_z(t)\dot{\theta}(t)\right]^2 dt = \ldots$$ $$= \int \left[\left(K_x x(t) + D_x \dot{x}(t)\right)\dot{x}(t)\right]^2 dt + \int \left[\left(K_y y(t) + D_y \dot{y}(t)\right)\dot{y}(t)\right]^2 dt + \int \left[\left(K_r \theta(t) + D_r \dot{\theta}(t)\right)\dot{\theta}(t)\right]^2 dt$$ $$J = w_{\min SEC}\left(E_c^{shank} + E_c^{femur} + E_c^{pelvis}\right) \qquad (14)$$

- Tracking terms:

Joint torques (Phases B, C1 and C2)	$$J = w_{trTh} \sum_{i}^{nTh} \left(\frac{T_i}{T_0} - u_{T_i}\right)^2 + w_{trTe} \sum_{i}^{nTe} \left(\frac{T_i}{T_0} - u_{T_i}\right)^2 \qquad (15)$$
Ground reaction forces (All phases)	$$J = w_{trGRF_x}\left(\frac{GRF_x/T_0 - u_{GRF_x}}{30}\right)^2 + w_{trGRF_y}\left(\frac{GRF_y/T_0}{30} - u_{GRF_y}\right)^2 + \ldots$$ $$\ldots + w_{trCOP}\left(\frac{COP_{x\,\mathrm{mod}} - COP_{x\,\mathrm{exp}}}{0.02}\right)^2$$ (16)
Coordinates (Phases A and B)	$$J = w_{trqh} \sum_{i}^{3} \left(\frac{q_i - q_{\mathrm{exp}\,i}}{0.02}\right)^2 + w_{trqe} \sum_{i}^{3} \left(\frac{q_i - q_{\mathrm{exp}\,i}}{0.02}\right)^2 \qquad (17)$$
Velocities (Phases A and B)	$$J = w_{trqh} \sum_{i}^{3} \left(\frac{\dot{q}_i - \dot{q}_{\mathrm{exp}\,i}}{0.05}\right)^2 + w_{trqe} \sum_{i}^{3} \left(\frac{\dot{q}_i - \dot{q}_{\mathrm{exp}\,i}}{0.05}\right)^2 \qquad (18)$$
Subject-exoskeleton contact forces (Phase B)	$$J = w_{trSE} \sum_{i}^{nSEC} \left(F_{\mathrm{mod}\,i}^{SEC} - F_{\mathrm{exp}\,i}^{SEC}\right)^2 \qquad (19)$$

with the weights $w_{\min T} = 1$, $w_{trTh} = 1$, $w_{trTe} = 10$, $w_{\min \dddot{q}} = 0.1$, $w_{trGRF_x} = 1$, $w_{trGRF_y} = 100$, $w_{trCOP} = 100$, $w_{trqh} = 0.1$, $w_{trqe} = 1$, $w_{trSE} = 1$, $w_{\min SEC} = 10$

2) Parameter identification analysis for foot-ground contact model

Following the method of Van den Hof et al. (*Model. Control Bridg. Rigorous Theory Adv. Technol.* 125: 125–143, 2009), the parameter identification consists of calculating the singular value decomposition of the second derivatives (Hessian matrix) of the contact force with respect to the parameters of the contact model.

Foot-ground contact model parameters

We used a compliant foot-ground contact model. The relation between those forces and kinematics is non-linear. The second derivative of the vertical contact force at the heel sphere with respect to the parameters of the model is the following:

$$H = \frac{\partial^2 GRF_v}{\partial w^2} \tag{20}$$

where GRF_v is the vertical component of the ground reaction force and *w* a vector containing the five parameters of the foot-ground contact model affecting this force: stiffness and damping parameters (equal for front and heel spheres), horizontal and vertical positions of the centre of the sphere with respect to calcaneus, and the radius of the sphere. The singular value decomposition results for *H* are the one shown in Figure S2.

The redundancy produced by two input variables with the same effect on the ground reaction force makes the convergence of the optimization difficult. The first unit vector shows that the vertical position of the spheres (y_{heel}) is coupled with the radius of the sphere (r_{heel}). This means that, for example, a decrease of y_{heel} would have the same effect as an increase of r_{heel}. This is true when considering that the foot orientation is flat with respect to the ground (the case in sit-to-stance movements).

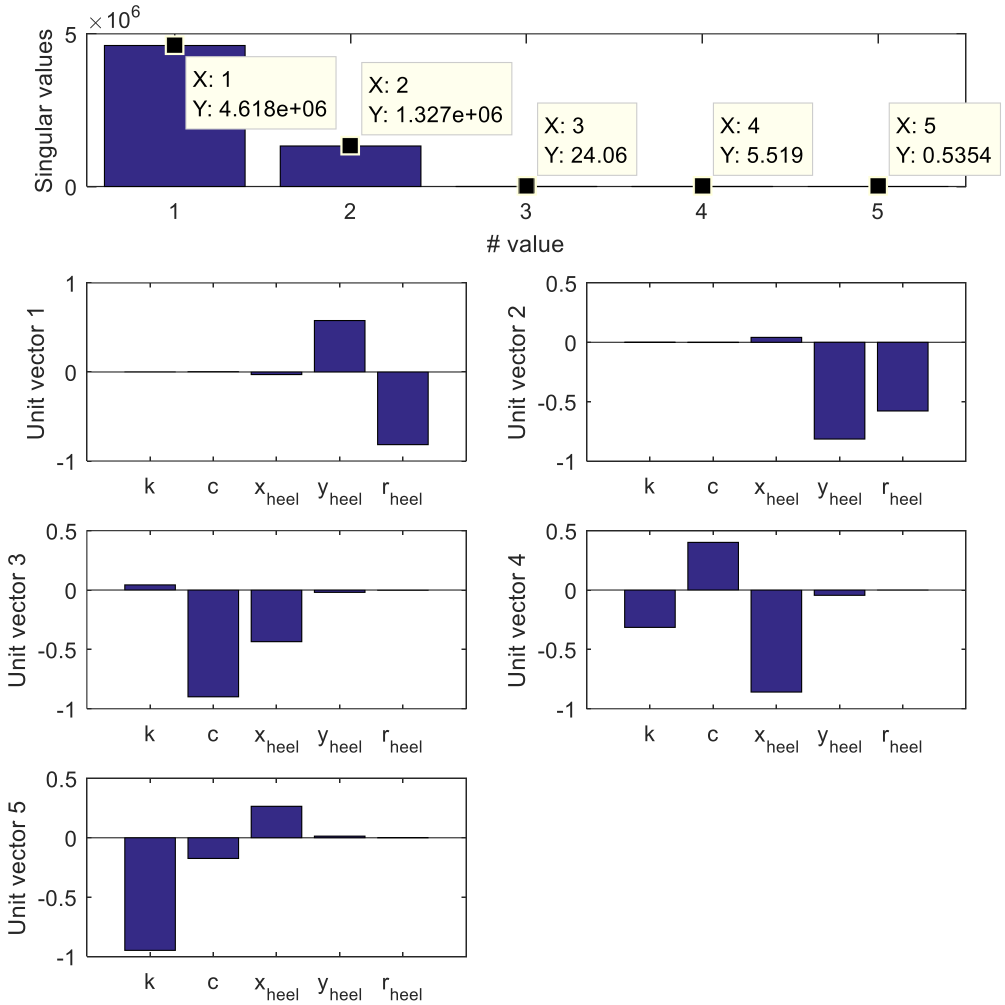

Figure S2. Singular value decomposition of the hessian matrix obtained as the second derivative of the vertical GRF with respect to the foot-ground contact parameters.

3) Values of the optimized parameters

Foot-ground contact parameters obtained in Phase A:

Stiffness *k*: $1.32 \cdot 10^7$ $[N/m^2]^{2/3}$	Damping *c*: 6.19 m^{-1}	See equations (2) and (3) from the Appendix 1
x_{heel} = -0.09 m	y_{heel} = 0.006 m	*x* and *y* coordinates are relative to the calcaneus frame
x_{front} = 0.30 m	y_{front} = 0.01 m	

Subject-exoskeleton contact parameters obtained in Phase B:

	Pelvis	**Thigh**	**Ankle**	
x (m)	3.9	0.0	-0.1	x and y coordinates are relative to the human pelvis, thigh or shank body respectively
y (m)	1.3	-4.8	-0.1	
K_{rz} [Nm/rad]	-9.7	-49.0	-7.5	
K_{tx} [N/m]	-0.6	-423.5	-1000	
K_{ty} [N/m]	-29.8	-0.8	1000	