Noname manuscript No.
(will be inserted by the editor)

Shape Optimization for a Link Mechanism

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Received: date / Accepted: date

Abstract This paper presents a numerical solution for shape optimization problems for link mechanisms, such as a piston-crank mechanism. The dynamic behavior of a link mechanism is described by a differential-algebraic equation (DAE) system consisting of motion equations for each single body and constraints of linkages and rigid motions. In a shape optimization problem, the objective function to maximize is constructed from the external work done by a given external force, which agrees with the kinetic energy of the link mechanism, for an assigned time interval, and the total volume of all the links forms the constraint function. The Fréchet derivatives of these cost functions with respect to the domain variation, which we call the shape derivatives of these cost functions, are evaluated theoretically. A scheme to solve the shape optimization problem is presented using the H^1 gradient method (the traction method) proposed by the authors as a reshaping algorithm, since it retains the smoothness of the boundary. A numerical example shows that reasonable shapes for each link such that mobility of the link mechanism is improved are obtained by this approach.

Keywords Shape optimization · Multibody system · Differential-algebraic equation (DAE) · Shape derivative · H^1 gradient method · Traction method

This paper was presented at CJK-OSM 7, June, 18-21, 2012, Huangshan, China.

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1 Introduction

Rigid bodies linked together at joints are called a link mechanism or a multibody system, and they are used as a mathematical model to analyze motion, such as for a machine or an animal with bones. The dynamic behavior of a multibody system is described by a differential-algebraic equation (DAE) system consisting of motion equations for each single body with constraints formed by the linkages and rigid motions. The solution of the DAE system has been studied extensively[2, 8, 7]. Based on the solution, many numerical analysis systems have been developed and used for the design of machines and for analysis of the motion of living things. However, the shapes of multibody systems have not been optimized by the use of a gradient-based method.

In the present paper, choosing a piston-crank mechanism as an example of a link mechanism, we formulate a shape optimization problem and formulate a numerical solution to it.

We discuss this as follows. In Section 2, we define the initial domains of the rigid bodies and choose as design variables the mappings from the initial domains to varied domains. Using the domains, in Section 3, we formulate the main problem of motion for a link mechanism. In Section 4, using the solution for the motion, we formulate a shape optimization problem using external work done by a given external force, which agrees with the kinetic energy of the link mechanism, as the objective function to maximize, and the total volume of the entire rigid body as a constraint function.

The evaluation methods for the Fréchet derivatives of the cost functions with respect to the domain variation, which we call the shape derivatives of the cost functions, are shown in Section 5. Using these shape derivatives of the cost functions, we present in Section

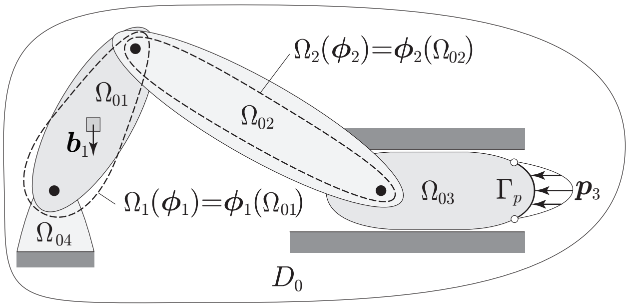


Fig. 1 Mappings ϕ_1 and ϕ_2 from initial domains Ω_{01} and Ω_{02} of linked rigid bodies at time $t = 0$

6 a method called the H^1 gradient method to obtain the domain mappings that decrease the cost functions.

An introduction of the H^1 gradient method is presented in the previous paper[4]. The main reason why we use this method is as follows. If we use boundary integral form for shape derivatives of cost functions, we obtain shape derivatives as functions defined on boundary with the unit outer normal. Since the normal is given by the derivative of the boundary shape, it has less smoothness than original smoothness of the boundary. To recover the lack of smoothness of the shape derivative, we use the H^1 gradient method. In this method, domain variation is obtained as a solution to a boundary value problem of an elliptic partial differential equation, such as a linear elastic problem defined in the original domain using the Neumann condition with the negative value of the shape derivative on the boundary. The smoothness of the solution on the boundary improves one time differentiability from the shape derivative.

A scheme to solve the shape optimization problem with constraints is presented in Section 7. Finally, in Section 8, we show the numerical result for shape optimization of a piston-crank mechanism.

2 Admissible set of design variables

Let us define the domains for the link mechanism depicted in Fig. 1. Let D_0 be a $d = 2$ dimensional bounded domain in which a link mechanism is allowed to be designed. We assume D_0 is fixed. Let $\mathcal{L} = \{1, 2, \cdots, |\mathcal{L}|\}$ denote a set of index numbers for the links. In the present paper, we use the notation $|\cdot|$ to denote the number of elements in a finite set.

For each $l \in \mathcal{L}$, let $\Omega_{0l} \subset D_0$ denote the initial domain for the l-th link. To simplify notation, we let Ω_0 represent $\left\{\Omega_{01}, \cdots, \Omega_{0|\mathcal{L}|}\right\}$. To define a shape optimization problem for Ω_0, its boundaries

$$\partial\Omega_0 = \left\{\partial\Omega_{01}, \cdots, \partial\Omega_{0|\mathcal{L}|}\right\}$$

are required to be at least the Lipschitz boundary, i.e., the $W^{1,\infty}$ class.

In the present paper, we use the notation

$$W^{s,p}\left(\Omega_{0l}; \mathbb{R}^d\right)$$

to denote the Sobolev space for the set of functions defined in Ω_{0l} and having values in $\mathbb{R}^d$ that are $s \in [0, \infty]$ times differentiable and $p \in [1, \infty]$-th order Lebesgue integrable, and call its smoothness the $W^{s,p}$ class. The notation $H^s\left(\Omega_{0l}; \mathbb{R}^d\right)$ is used as $W^{s,2}\left(\Omega_{0l}; \mathbb{R}^d\right)$. In the present paper, since we use boundary integral formulae for shape derivatives, we assume $\partial\Omega_0$ is the piecewise C^1 class to define the normal $\boldsymbol{\nu}$. We denote by $\partial\Omega_0^-$ the open sets on $\partial\Omega_0$ except the sets of measure 0, which are not contained in the C^1 class. We assume that $\Gamma_{p0} \subset \partial\Omega_0$ is a boundary on which external force acts, and Γ_{p0} is of the C^2 class on $\Gamma_{p0} \cap \partial\Omega_0^-$ to define the curvature $\kappa = \boldsymbol{\nabla} \cdot \boldsymbol{\nu}$ in Eq. (55).

For each $l \in \mathcal{L}$, let $\boldsymbol{\phi}_l = (\phi_{l1}, \cdots, \phi_{ld})^{\mathrm{T}} : D_0 \to \mathbb{R}^d$ be the domain mapping from the initial domain $\Omega_{0l} \subset D_0$ belonging to $W^{1,\infty}\left(D_0; \mathbb{R}^d\right)$ because of maintaining the Lipschitz boundary in the new domain. For each $l \in \mathcal{L}$, let

$$\boldsymbol{F}(\boldsymbol{\phi}_l) = \boldsymbol{\phi}_{l\boldsymbol{x}^{\mathrm{T}}} = \left(\frac{\partial \phi_{li}}{\partial x_j}\right) \in L^\infty\left(D_0; \mathbb{R}^{d\times d}\right), \tag{1}$$

$$\omega(\boldsymbol{\phi}_l) = \det \boldsymbol{F}(\boldsymbol{\phi}_l) \in L^\infty(D_0; \mathbb{R}) \tag{2}$$

be the Jacobi matrix and the Jacobian of $\boldsymbol{\phi}_l$ with respect to $\boldsymbol{x} \in D_0$, respectively. In the present paper, let $(\,\cdot\,)^{\mathrm{T}}$ denote the transpose, and $(\,\cdot\,)_{\boldsymbol{x}}$ denote $\partial(\,\cdot\,)/\partial\boldsymbol{x}$. We define

$$V = \left\{\boldsymbol{\phi} \in W^{1,\infty}\left(D_0; \mathbb{R}^d\right) \;\middle|\; \operatorname*{ess\,inf}_{\boldsymbol{x}\in\Omega_0} \omega_0(\boldsymbol{\phi}) > 0\right\} \tag{3}$$

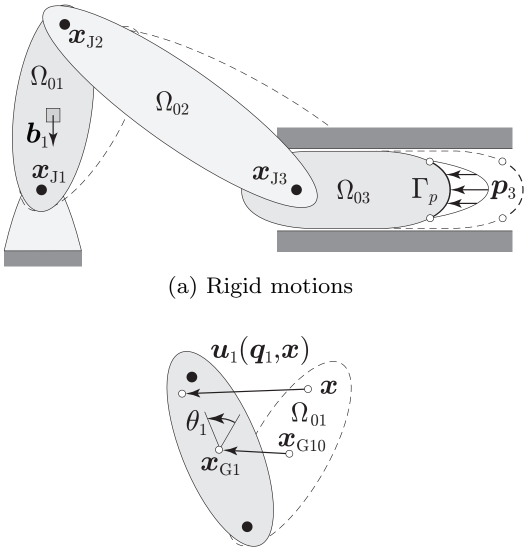
as a Banach space with the norm of $W^{1,\infty}\left(D_0;\ \mathbb{R}^d\right)$ for each $\boldsymbol{\phi}_l$, $l \in \mathcal{L}$. V is used to define the Fréchet derivatives with respect to the domain variation. Moreover, we assume that the admissible set for each $\boldsymbol{\phi}_l$, $l \in \mathcal{L}$, is defined as

$$\mathcal{C}_l = \Big\{\boldsymbol{\phi}_l \in V \;\Big|\; \|\boldsymbol{\phi}_l - \boldsymbol{\phi}_0\|_V < 1,\ \boldsymbol{\phi}_l(\Omega_{0l}) \subseteq D_0, \\ C^1 \text{ class on } \partial\Omega_0^-,\, C^2 \text{ class on } \Gamma_{p0} \cap \partial\Omega_0^-\Big\}, \tag{4}$$

where $\boldsymbol{\phi}_0$ is an identity mapping, e.g., $\boldsymbol{\phi}_0(\boldsymbol{x}) = \boldsymbol{x}$ for $\boldsymbol{x} \in D_0$. $\|\boldsymbol{\phi}_l - \boldsymbol{\phi}_0\|_V < 1$ is used so that $\boldsymbol{\phi}_l \in \mathcal{C}_l$ is a one-to-one mapping. We use the notation $\Omega_l(\boldsymbol{\phi}_l) = \boldsymbol{\phi}_l(\Omega_{0l})$, $\Gamma_{pl}(\boldsymbol{\phi}_l) = \boldsymbol{\phi}_l(\Gamma_{p0})$, etc., for $\boldsymbol{\phi}_l \in \mathcal{C}_l$. To simplify notation, we denote

$$\boldsymbol{\phi} = \left(\boldsymbol{\phi}_1, \cdots, \boldsymbol{\phi}_{|\mathcal{L}|}\right)^{\mathrm{T}} \in \mathcal{C} = \mathcal{C}_1 \times \cdots \times \mathcal{C}_{|\mathcal{L}|}, \tag{5}$$

$$\Omega(\boldsymbol{\phi}) = \left\{\Omega_1(\boldsymbol{\phi}_1), \cdots, \Omega_{|\mathcal{L}|}\left(\boldsymbol{\phi}_{|\mathcal{L}|}\right)\right\}. \tag{6}$$



(a) Rigid motions

(b) Displacement by rigid motion of Ω_{01}

Fig. 2 Link mechanism

3 Main problem

Using the definition of domains, let us define the motion of a link mechanism. We assume that the domains of the link mechanism are defined at time $t = 0$, and that a volume force $\boldsymbol{b}_l$ and a boundary force $\boldsymbol{p}_l$ applied to the l-th link move a link mechanism as shown in Fig. 2 during time $(0, t_1)$ with positive constant t_1.

Definition 1 (Rigid motions) For $l \in \mathcal{L}$, let $\boldsymbol{x}_{\mathrm{G}l0}$ denote the position of the center of mass for the l-th link at $t = 0$, and let $\boldsymbol{x}_{\mathrm{G}l} : (0, t_1) \to \mathbb{R}^d$ and $\theta_l : (0, t_1) \to \mathbb{R}$ denote the position of the center of mass for the l-th link and the rotation around $\boldsymbol{x}_{\mathrm{G}l0}$, respectively. For $t \in (0, t_1)$, we call

$$\boldsymbol{q}_l(t) = \left((\boldsymbol{x}_{\mathrm{G}l}(t) - \boldsymbol{x}_{\mathrm{G}l0})^{\mathrm{T}}, \theta_l(t) \right)^{\mathrm{T}} \in \mathbb{R}^{d_{\mathrm{F}}}$$

the rigid motion of the l-th link and

$$\boldsymbol{q} = \left(\boldsymbol{q}_1^{\mathrm{T}}, \cdots, \boldsymbol{q}_{|\mathcal{L}|}^{\mathrm{T}} \right)^{\mathrm{T}} : (0, t_1) \to \boldsymbol{q}_l \in \mathbb{R}^{d_{\mathrm{F}}|\mathcal{L}|}$$

the total rigid motion. Here, $d_{\mathrm{F}} = 3$ denotes the degrees of freedom of a link.

From $\boldsymbol{q}_l$, displacement at all points in $\Omega_l(\boldsymbol{\phi}_l)$ can be computed as follows.

Definition 2 (Displacement by rigid motion) For $l \in \mathcal{L}$, $t \in (0, t_1)$, and $\boldsymbol{x} \in \Omega_l(\boldsymbol{\phi}_l)$,

$$\boldsymbol{u}_l(\boldsymbol{q}_l, \boldsymbol{x}) = \boldsymbol{x}_{\mathrm{G}l}(t) - \boldsymbol{x}_{\mathrm{G}l}(0) + \theta_l(t)\, \boldsymbol{e}_3 \times (\boldsymbol{x} - \boldsymbol{x}_{\mathrm{G}l}(0))$$

is called the displacement by rigid motion $\boldsymbol{q}_l$, where $\boldsymbol{e}_3 \in \mathbb{R}^3$ denotes the unit vector in the direction of the x_3 axis.

Using the displacement, the motion constraints will be denoted as follows. Let $\mathcal{J} = \{1, 2, \cdots, |\mathcal{J}|\}$ be a set of indices for the linkage conditions. In the same manner, let $\mathcal{T} = \{1, 2, \cdots, |\mathcal{T}|\}$ and $\mathcal{R} = \{1, 2, \cdots, |\mathcal{R}|\}$ be the sets of indices for the rigid-motion constraints of translation and rotation, respectively.

Definition 3 (Motion constraints) For each $k \in \mathcal{J}$, let $\boldsymbol{x}_{\mathrm{J}k} \in \Omega_l(\boldsymbol{\phi}_l) \cap \Omega_m(\boldsymbol{\phi}_m)$ be the linkage points for the k-th linkage condition between the $l \in \mathcal{L}$-th and $m \in \mathcal{L}$-th links such that $l \neq m$, and $\boldsymbol{u}_l(\boldsymbol{q}_l, \boldsymbol{x})$ and $\boldsymbol{u}_m(\boldsymbol{q}_m, \boldsymbol{x})$ are the displacements of the l-th and m-th links. We call

$$\boldsymbol{u}_l(\boldsymbol{q}_l, \boldsymbol{x}_{\mathrm{J}k}) - \boldsymbol{u}_m(\boldsymbol{q}_m, \boldsymbol{x}_{\mathrm{J}k}) = \boldsymbol{0} \in \mathbb{R}^d \tag{7}$$

the k-th linkage constraint, and write (7) for $k \in \mathcal{J}$ as

$$\boldsymbol{\psi}_{\mathrm{J}k}(\boldsymbol{q}) = (\psi_{\mathrm{J}k1}(\boldsymbol{q}), \cdots, \psi_{\mathrm{J}kd}(\boldsymbol{q}))^{\mathrm{T}} = \boldsymbol{0} \in \mathbb{R}^d.$$

For the constraints of rigid motions, we write

$$\psi_{\mathrm{T}k}(\boldsymbol{q}) = 0 \in \mathbb{R}$$

for translation $k \in \mathcal{T}$ and

$$\psi_{\mathrm{R}k}(\boldsymbol{q}) = 0 \in \mathbb{R}$$

for rotation $k \in \mathcal{R}$. Combining these constraints, we call

$$\begin{aligned}\boldsymbol{\psi}(\boldsymbol{q}) = \Big(&\psi_{\mathrm{J}11}(\boldsymbol{q}), \cdots, \psi_{\mathrm{J}|\mathcal{J}|d}^{\mathrm{T}}(\boldsymbol{q}), \\ &\psi_{\mathrm{T}1}(\boldsymbol{q}), \cdots, \psi_{\mathrm{T}|\mathcal{T}|}(\boldsymbol{q}), \psi_{\mathrm{R}1}(\boldsymbol{q}), \cdots, \psi_{\mathrm{R}|\mathcal{R}|}(\boldsymbol{q}) \Big)^{\mathrm{T}} \\ = \boldsymbol{0} \in \mathbb{R}^{d|\mathcal{J}|+|\mathcal{T}|+|\mathcal{R}|}\end{aligned} \tag{8}$$

the motion constraints of the global system.

In the present paper, let $(\dot{\,\cdot\,})$ denote $\partial(\,\cdot\,)/\partial t$. Here, we define notations for the derivatives of $\boldsymbol{\psi}(\boldsymbol{q})$ as

$$\dot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}}] = \boldsymbol{\psi}'(\boldsymbol{q})[\dot{\boldsymbol{q}}], \tag{9}$$

$$\ddot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}}, \ddot{\boldsymbol{q}}] = \boldsymbol{\psi}''(\boldsymbol{q})[\dot{\boldsymbol{q}}, \dot{\boldsymbol{q}}] + \boldsymbol{\psi}'(\boldsymbol{q})[\ddot{\boldsymbol{q}}], \tag{10}$$

where

$$\boldsymbol{\psi}'(\boldsymbol{q})[\boldsymbol{r}] = \frac{\partial \boldsymbol{\psi}}{\partial \boldsymbol{q}^{\mathrm{T}}}(\boldsymbol{q}) \cdot \boldsymbol{r}, \tag{11}$$

$$\boldsymbol{\psi}''(\boldsymbol{q})[\boldsymbol{r}, \boldsymbol{t}] = \frac{\partial}{\partial \boldsymbol{q}^{\mathrm{T}}} \left(\frac{\partial \boldsymbol{\psi}}{\partial \boldsymbol{q}^{\mathrm{T}}}(\boldsymbol{q}) \cdot \boldsymbol{r} \right) \cdot \boldsymbol{t}, \tag{12}$$

for $\boldsymbol{r}, \boldsymbol{t} \in \mathbb{R}^{d_{\mathrm{F}}|\mathcal{L}|}$. Then, (8) is equivalent to

$$\ddot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}}, \ddot{\boldsymbol{q}}] = \boldsymbol{0} \quad \text{in } (0, t_1), \tag{13}$$

$$\dot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}}] = \boldsymbol{0} \quad \text{in } (0, t_1), \tag{14}$$

$$\dot{\boldsymbol{\psi}}(\boldsymbol{q}(0))[\dot{\boldsymbol{q}}(0)] = \boldsymbol{0}, \tag{15}$$

$$\boldsymbol{\psi}(\boldsymbol{q}(0)) = \boldsymbol{0}. \tag{16}$$

The generalized mass can be defined as follows.

Definition 4 (Generalized mass) For $l \in \mathcal{L}$, let $\rho_l \in W^{1,\infty}(D_0;\mathbb{R})$, $\rho_l > 0$, be the density in the l-th link. We call

$$\boldsymbol{M}(\boldsymbol{\phi}) = \operatorname{diag}\Big(m_1(\boldsymbol{\phi}_1), m_1(\boldsymbol{\phi}_1), j_{\mathrm{G}1}(\boldsymbol{\phi}_1),\\ \cdots, m_{|\mathcal{L}|}(\boldsymbol{\phi}_{|\mathcal{L}|}), m_{|\mathcal{L}|}(\boldsymbol{\phi}_{|\mathcal{L}|}), j_{\mathrm{G}|\mathcal{L}|}(\boldsymbol{\phi}_{|\mathcal{L}|})\Big)$$

the generalized mass, where

$$m_l(\boldsymbol{\phi}_l) = \int_{\Omega_l(\boldsymbol{\phi}_l)} \rho_l \,\mathrm{d}x,$$
$$j_{\mathrm{G}l}(\boldsymbol{\phi}_l) = \int_{\Omega_l(\boldsymbol{\phi}_l)} \rho_l \|\boldsymbol{x} - \boldsymbol{x}_{\mathrm{G}l}(0)\|^2_{\mathbb{R}^d} \,\mathrm{d}x.$$

The generalized external force can be defined as follows. For $l \in \mathcal{L}$, let

$$\tilde{\Omega}_l(\boldsymbol{\phi}_l, \boldsymbol{q}_l) = \{\boldsymbol{x} + \boldsymbol{u}_l(\boldsymbol{q}_l, \boldsymbol{x}) \mid \boldsymbol{x} \in \Omega_l(\boldsymbol{\phi}_l)\},$$
$$\tilde{\Gamma}_{pl}(\boldsymbol{\phi}_l, \boldsymbol{q}_l) = \{\boldsymbol{x} + \boldsymbol{u}_l(\boldsymbol{q}_l, \boldsymbol{x}) \mid \boldsymbol{x} \in \partial\Omega_l(\boldsymbol{\phi}_l) \cap \Gamma_p(\boldsymbol{\phi}_l)\}.$$

Definition 5 (Generalized external force) For $l \in \mathcal{L}$, let $\boldsymbol{b}_l : (0,t_1) \to W^{1,\infty}(D_0;\mathbb{R}^d)$ and $\boldsymbol{p}_l : (0,t_1) \to W^{2,\infty}(D_0;\mathbb{R}^d)$ be the volume force applied to the l-th link, and the boundary force applied for $\partial\Omega_l(\boldsymbol{\phi}_l) \cap \Gamma_{pl}(\boldsymbol{\phi}_l)$, respectively. We call

$$\boldsymbol{s}_l(\boldsymbol{\phi}_l, \boldsymbol{q}_l, \boldsymbol{b}_l, \boldsymbol{p}_l)\\ = \left(\boldsymbol{s}^{\mathrm{T}}_{\mathrm{F}l}(\boldsymbol{\phi}_l, \boldsymbol{q}_l, \boldsymbol{b}_l, \boldsymbol{p}_l), s_{\mathrm{M}l}(\boldsymbol{\phi}_l, \boldsymbol{q}_l, \boldsymbol{b}_l, \boldsymbol{p}_l)\right)^{\mathrm{T}} \in \mathbb{R}^{d_{\mathrm{F}}}$$

the generalized external force applied to the l-th link, where

$$\boldsymbol{s}_{\mathrm{F}l}(\boldsymbol{\phi}_l, \boldsymbol{q}_l, \boldsymbol{b}_l, \boldsymbol{p}_l) = \int_{\tilde{\Omega}_l(\boldsymbol{\phi}_l, \boldsymbol{q}_l)} \boldsymbol{b}_l(t) \,\mathrm{d}x\\ + \int_{\tilde{\Gamma}_{pl}(\boldsymbol{\phi}_l, \boldsymbol{q}_l)} \boldsymbol{p}_l(t) \,\mathrm{d}\gamma \in \mathbb{R}^d,$$
$$s_{\mathrm{M}l}(\boldsymbol{\phi}_l, \boldsymbol{q}_l, \boldsymbol{b}_l, \boldsymbol{p}_l)\boldsymbol{e}_3\\ = \int_{\tilde{\Omega}_l(\boldsymbol{\phi}_l, \boldsymbol{q}_l)} \boldsymbol{b}_l(t) \times (\boldsymbol{x} - \boldsymbol{x}_{\mathrm{G}l}(t)) \,\mathrm{d}x\\ + \int_{\tilde{\Gamma}_{pl}(\boldsymbol{\phi}_l, \boldsymbol{q}_l)} \boldsymbol{p}_l(t) \times (\boldsymbol{x} - \boldsymbol{x}_{\mathrm{G}l}(t)) \,\mathrm{d}\gamma \in \mathbb{R}^3.$$

To simplify notation, we denote

$$\boldsymbol{b} = \left(\boldsymbol{b}^{\mathrm{T}}_1, \cdots, \boldsymbol{b}^{\mathrm{T}}_{|\mathcal{L}|}\right)^{\mathrm{T}},$$
$$\boldsymbol{p} = \left(\boldsymbol{p}^{\mathrm{T}}_1, \cdots, \boldsymbol{p}^{\mathrm{T}}_{|\mathcal{L}|}\right)^{\mathrm{T}}$$

and call $\boldsymbol{s}(\boldsymbol{\phi}, \boldsymbol{q}, \boldsymbol{b}, \boldsymbol{p}) = \left(\boldsymbol{s}^{\mathrm{T}}_1, \cdots, \boldsymbol{s}^{\mathrm{T}}_{|\mathcal{L}|}\right)^{\mathrm{T}}$ the general force of the global system.

Based upon the above definitions, the problem of finding the rigid motion that satisfies the motion constraints can be written as follows.

Problem 1 (Main problem) Let $\boldsymbol{b}$ and $\boldsymbol{p}$ be given as in Definition 5. Let $\boldsymbol{q}_0$ and $\boldsymbol{q}_1 \in \mathbb{R}^{d_{\mathrm{F}}|\mathcal{L}|}$ be constants for initial conditions of $\boldsymbol{q}$ and $\dot{\boldsymbol{q}}$ at $t = 0$ such that

$$\dot{\boldsymbol{\psi}}(\boldsymbol{q}_0)[\boldsymbol{q}_1] = \boldsymbol{0}, \tag{17}$$
$$\boldsymbol{\psi}(\boldsymbol{q}_0) = \boldsymbol{0}. \tag{18}$$

For some $\boldsymbol{\phi} \in \mathcal{C}$ defined in (5), let $\boldsymbol{\psi}(\boldsymbol{q})$, $\boldsymbol{M}(\boldsymbol{\phi})$, and $\boldsymbol{s}(\boldsymbol{\phi}, \boldsymbol{q}, \boldsymbol{b}, \boldsymbol{p})$ be as in Definitions 3, 4, and 5, respectively. Find $\boldsymbol{q} \in H^1\left((0,t_1);\mathbb{R}^{d_{\mathrm{F}}|\mathcal{L}|}\right)$ such that

$$\boldsymbol{M}(\boldsymbol{\phi})\ddot{\boldsymbol{q}} = \boldsymbol{s}(\boldsymbol{\phi}, \boldsymbol{q}, \boldsymbol{b}, \boldsymbol{p}) \quad \text{in } (0,t_1), \tag{19}$$
$$\ddot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}}, \ddot{\boldsymbol{q}}] = \boldsymbol{0} \quad \text{in } (0,t_1), \tag{20}$$
$$\dot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}}] = \boldsymbol{0} \quad \text{in } (0,t_1), \tag{21}$$
$$\dot{\boldsymbol{q}}(0) = \boldsymbol{q}_1, \tag{22}$$
$$\boldsymbol{q}(0) = \boldsymbol{q}_0. \tag{23}$$

Here, we introduce

$$\boldsymbol{\mu} = \Big(\mu_{\mathrm{J}11}, \cdots, \mu_{\mathrm{J}|\mathcal{J}|d}, \mu_{\mathrm{T}1}, \cdots, \mu_{\mathrm{T}|\mathcal{T}|}, \mu_{\mathrm{R}1},\\ \cdots, \mu_{\mathrm{R}|\mathcal{R}|}\Big)^{\mathrm{T}} \in H^1\left((0,t_1);\mathbb{R}^{d|\mathcal{J}|+|\mathcal{T}|+|\mathcal{R}|}\right)$$

such that

$$\boldsymbol{\mu}(t_1) = \boldsymbol{0}, \tag{24}$$

as the Lagrange multipliers for (20). At the same time, we consider $\dot{\boldsymbol{\mu}}$ as the Lagrange multipliers for (21). Moreover, we introduce $\boldsymbol{r} \in H^1\left((0,t_1);\mathbb{R}^{d_{\mathrm{F}}|\mathcal{L}|}\right)$ as an adjoint function for $\boldsymbol{q}$ satisfying

$$\ddot{\boldsymbol{\psi}}(\boldsymbol{r})[\dot{\boldsymbol{r}}, \ddot{\boldsymbol{r}}] = \boldsymbol{0} \quad \text{in } (0,t_1), \tag{25}$$
$$\dot{\boldsymbol{\psi}}(\boldsymbol{r})[\dot{\boldsymbol{r}}] = \boldsymbol{0} \quad \text{in } (0,t_1), \tag{26}$$
$$\dot{\boldsymbol{r}}(t_1) = \dot{\boldsymbol{q}}(t_1), \tag{27}$$
$$\boldsymbol{r}(t_1) = \boldsymbol{q}(t_1). \tag{28}$$

For the motion constraints of the adjoint function given by (25), we introduce

$$\boldsymbol{\eta} = \Big(\eta_{\mathrm{J}11}, \cdots, \eta_{\mathrm{J}|\mathcal{J}|d}, \eta_{\mathrm{T}1}, \cdots, \eta_{\mathrm{T}|\mathcal{T}|}, \eta_{\mathrm{R}1},\\ \cdots, \eta_{\mathrm{R}|\mathcal{R}|}\Big)^{\mathrm{T}} \in H^1\left((0,t_1);\mathbb{R}^{d|\mathcal{J}|+|\mathcal{T}|+|\mathcal{R}|}\right)$$

such that

$$\boldsymbol{\eta}(0) = \boldsymbol{0} \tag{29}$$

as the Lagrange multipliers. At the same time, we consider $\dot{\boldsymbol{\eta}}$ as the Lagrange multipliers for (26). Then the simultaneous equations of the variational form of the motion equations (19) combined with the variational form of (26) with the Lagrange multipliers $\dot{\boldsymbol{\eta}}$ and the variational form of the motion constraints (20) can be written as

$$\int_0^{t_1}\left(\begin{pmatrix}\boldsymbol{M}(\boldsymbol{\phi}) & \boldsymbol{0} & \boldsymbol{0}\\ \boldsymbol{0} & \boldsymbol{M}(\boldsymbol{\phi}) & \left(\boldsymbol{\psi}_{\boldsymbol{q}^{\mathrm{T}}}(\boldsymbol{q})\right)^{\mathrm{T}}\\ \boldsymbol{0} & \boldsymbol{\psi}_{\boldsymbol{q}^{\mathrm{T}}}(\boldsymbol{q}) & \boldsymbol{0}\end{pmatrix}\begin{pmatrix}\dot{\boldsymbol{q}}\\ \ddot{\boldsymbol{q}}\\ \dot{\boldsymbol{\eta}}\end{pmatrix} + \begin{pmatrix}\boldsymbol{0} & -\boldsymbol{M}(\boldsymbol{\phi}) & \boldsymbol{0}\\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0}\\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0}\end{pmatrix}\begin{pmatrix}\boldsymbol{q}\\ \dot{\boldsymbol{q}}\\ \boldsymbol{\eta}\end{pmatrix}\right)\cdot\begin{pmatrix}\boldsymbol{r}\\ \dot{\boldsymbol{r}}\\ \boldsymbol{\mu}\end{pmatrix}\mathrm{d}t = \int_0^{t_1}\begin{pmatrix}\boldsymbol{0}\\ \boldsymbol{s}(\boldsymbol{\phi},\boldsymbol{q},\boldsymbol{b},\boldsymbol{p})\\ -\boldsymbol{\psi}''(\boldsymbol{q})[\dot{\boldsymbol{q}},\dot{\boldsymbol{q}}]\end{pmatrix}\cdot\begin{pmatrix}\boldsymbol{r}\\ \dot{\boldsymbol{r}}\\ \boldsymbol{\mu}\end{pmatrix}\mathrm{d}t. \tag{30}$$

The initial conditions of (22), (23), and (29) can be written as

$$\begin{pmatrix}\boldsymbol{q}(0)\\ \dot{\boldsymbol{q}}(0)\\ \boldsymbol{\eta}(0)\end{pmatrix} = \begin{pmatrix}\boldsymbol{q}_0\\ \boldsymbol{q}_1\\ \boldsymbol{0}\end{pmatrix}. \tag{31}$$

On the other hand, the terminal conditions of (27), (28), and (24) can be written as

$$\begin{pmatrix}\boldsymbol{r}(t_1)\\ \dot{\boldsymbol{r}}(t_1)\\ \boldsymbol{\mu}(t_1)\end{pmatrix} = \begin{pmatrix}\boldsymbol{q}(t_1)\\ \dot{\boldsymbol{q}}(t_1)\\ \boldsymbol{0}\end{pmatrix}. \tag{32}$$

If we denote

$$\boldsymbol{y} = \left(\boldsymbol{q}^{\mathrm{T}},\dot{\boldsymbol{q}}^{\mathrm{T}},\boldsymbol{\eta}^{\mathrm{T}}\right)^{\mathrm{T}},$$
$$\boldsymbol{z} = \left(\boldsymbol{r}^{\mathrm{T}},\dot{\boldsymbol{r}}^{\mathrm{T}},\boldsymbol{\mu}^{\mathrm{T}}\right)^{\mathrm{T}},$$

we can then write (30), (31), and (32) as

$$\int_0^{t_1}\left(\boldsymbol{A}(\boldsymbol{\phi},\boldsymbol{q})\dot{\boldsymbol{y}} + \boldsymbol{B}(\boldsymbol{\phi})\boldsymbol{y}\right)\cdot\boldsymbol{z}\,\mathrm{d}t = \int_0^{t_1}\boldsymbol{h}(\boldsymbol{\phi},\boldsymbol{q},\boldsymbol{b},\boldsymbol{p})\cdot\boldsymbol{z}\,\mathrm{d}t, \tag{33}$$

$$\boldsymbol{y}(0) = \boldsymbol{y}_0, \tag{34}$$

$$\boldsymbol{z}(t_1) = \boldsymbol{y}(t_1). \tag{35}$$

and the variational forms of (21) and (25) with the Lagrange multipliers $\dot{\boldsymbol{\mu}}$ and $\boldsymbol{\eta}$, respectively, as

$$\int_0^{t_1}\dot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}}]\cdot\dot{\boldsymbol{\mu}}\,\mathrm{d}t = 0, \tag{36}$$

$$\int_0^{t_1}\ddot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{r}},\ddot{\boldsymbol{r}}]\cdot\boldsymbol{\eta}\,\mathrm{d}t = 0. \tag{37}$$

Combining the equations from (33) to (37), we define the Lagrangian for Problem 1 as

$$\mathscr{L}_{\mathrm{MD}}(\boldsymbol{\phi},\boldsymbol{y},\boldsymbol{z}) = \int_0^{t_1}\Big\{\Big(-\boldsymbol{A}(\boldsymbol{\phi},\boldsymbol{q})\dot{\boldsymbol{y}} - \boldsymbol{B}(\boldsymbol{\phi})\boldsymbol{y} + \boldsymbol{h}(\boldsymbol{\phi},\boldsymbol{q},\boldsymbol{b},\boldsymbol{p})\Big)\cdot\boldsymbol{z} + \dot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}}]\cdot\dot{\boldsymbol{\mu}} + \ddot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{r}},\ddot{\boldsymbol{r}}]\cdot\boldsymbol{\eta}\Big\}\,\mathrm{d}t. \tag{38}$$

Here, $\boldsymbol{y} = \left(\boldsymbol{q}^{\mathrm{T}},\dot{\boldsymbol{q}}^{\mathrm{T}},\boldsymbol{\eta}^{\mathrm{T}}\right)^{\mathrm{T}}$ and $\boldsymbol{z} = \left(\boldsymbol{r}^{\mathrm{T}},\dot{\boldsymbol{r}}^{\mathrm{T}},\boldsymbol{\mu}^{\mathrm{T}}\right)^{\mathrm{T}}$ are arbitrary elements of

$$Y = \left\{\boldsymbol{y}\in H^1\left((0,t_1);\mathbb{R}^n\right)\big|\ \boldsymbol{y}(0) = \boldsymbol{0}\right\}, \tag{39}$$

$$Z = \left\{\boldsymbol{z}\in H^1\left((0,t_1);\mathbb{R}^n\right)\big|\ \boldsymbol{z}(t_1) = \boldsymbol{0}\right\}, \tag{40}$$

respectively, where $n = 2d_{\mathrm{F}}|\mathcal{L}| + d|\mathcal{J}| + |\mathcal{T}| + |\mathcal{R}|$. Moreover, recalling the definitions of $\boldsymbol{A}(\boldsymbol{\phi},\boldsymbol{q})$, $\boldsymbol{B}(\boldsymbol{\phi})$ and $\boldsymbol{h}(\boldsymbol{\phi},\boldsymbol{q},\boldsymbol{b},\boldsymbol{p})$, and using the notations from (9) to (12), (38) is written as

$$\mathscr{L}_{\mathrm{MD}}(\boldsymbol{\phi},\boldsymbol{y},\boldsymbol{z}) = \int_0^{t_1}\Big\{\Big(-\boldsymbol{M}\ddot{\boldsymbol{q}} - \left(\boldsymbol{\psi}_{\boldsymbol{q}^{\mathrm{T}}}(\boldsymbol{q})\right)^{\mathrm{T}}\dot{\boldsymbol{\eta}} + \boldsymbol{s}(\boldsymbol{\phi},\boldsymbol{q},\boldsymbol{b},\boldsymbol{p})\Big)\cdot\dot{\boldsymbol{r}} - \ddot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}},\ddot{\boldsymbol{q}}]\cdot\boldsymbol{\mu} + \dot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}}]\cdot\dot{\boldsymbol{\mu}} + \ddot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{r}},\ddot{\boldsymbol{r}}]\cdot\boldsymbol{\eta}\Big\}\,\mathrm{d}t. \tag{41}$$

Here, we used the conditions at $t = 0$ and $t = t_1$.

Using the above definitions, the variational form of Problem 1 can be written as follows.

Problem 2 (Variational form of Problem 1) Under the conditions given in Problem 1, let (33) and (34) denote (30) and (31). Find $\boldsymbol{y}$ such that $\boldsymbol{y} - \bar{\boldsymbol{y}} \in Y$ satisfies

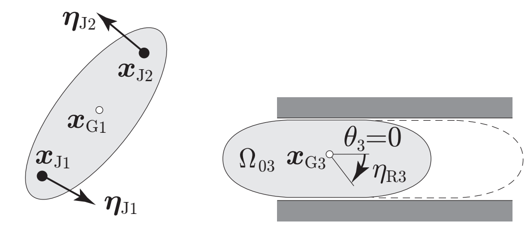
$$\mathscr{L}_{\mathrm{MD}}(\boldsymbol{\phi},\boldsymbol{y},\boldsymbol{z}) = 0$$

for all $\boldsymbol{z} = \left(\boldsymbol{r}^{\mathrm{T}},\dot{\boldsymbol{r}}^{\mathrm{T}},\boldsymbol{\mu}^{\mathrm{T}}\right)^{\mathrm{T}}$ such that $\boldsymbol{z} - \bar{\boldsymbol{z}} \in Z$. Here, $\bar{\boldsymbol{y}}$ is a function satisfying $\bar{\boldsymbol{y}}(0) = \boldsymbol{y}_0$, where $\boldsymbol{q}_0$ and $\boldsymbol{q}_1$ are functions satisfying (17) and (18). $\bar{\boldsymbol{z}}$ is a function satisfying $\bar{\boldsymbol{z}}(t_1) = \boldsymbol{y}(t_1)$. Y and Z are defined in (39) and (40), respectively.

For Problem 2, we can use a numerical solution as follows. From the variational form in Problem 2, we have the ordinary differential equation as

$$\boldsymbol{A}(\boldsymbol{\phi},\boldsymbol{q})\dot{\boldsymbol{y}} + \boldsymbol{B}(\boldsymbol{\phi})\boldsymbol{y} = \boldsymbol{h}(\boldsymbol{\phi},\boldsymbol{q},\boldsymbol{b},\boldsymbol{p}).$$

This equation system can be solved by a numerical integration scheme such as the Runge-Kutta method using the initial condition (34). In the solution, the Lagrange multipliers $\boldsymbol{\eta}_{\mathrm{J}i}$, $\eta_{\mathrm{T}j}$, and $\eta_{\mathrm{R}k}$ represent the linkage forces of the $i\in\mathcal{J}$-th constraint as shown in Fig. 3 (a), the correction force for the $j\in\mathcal{T}$-th translational rigid-motion constraint, and the correction moment for the $k\in\mathcal{R}$-th rotational rigid-motion constraint as shown in Fig. 3 (b), respectively.



(a) Linkage forces (b) Correction moment

Fig. 3 Linkage forces and correction forces

4 Shape optimization problem

Using the solution $\boldsymbol{y}$ to Problem 2, we define the cost functions as follows.

Definition 6 (Cost functions) Let $\boldsymbol{y}$ be the solution to Problem 2 for $\boldsymbol{\phi}_l \in \mathcal{C}_l$, $l \in \mathcal{L}$. We call

$$f_0(\boldsymbol{\phi}, \boldsymbol{y}) = -\int_0^{t_1} \boldsymbol{s}(\boldsymbol{\phi}, \boldsymbol{q}, \boldsymbol{b}, \boldsymbol{p}) \cdot \dot{\boldsymbol{q}} \, \mathrm{d}t, \tag{42}$$

$$f_1(\boldsymbol{\phi}) = c_1 - \sum_{l \in \mathcal{L}} \int_{\Omega_l(\boldsymbol{\phi}_l)} \mathrm{d}x \tag{43}$$

the objective and constraint functions, respectively; both functions are cost functions. f_0 consists of the negative-signed external work done by a given external forces $\boldsymbol{b}$ and $\boldsymbol{p}$, which agrees with the negative-signed kinetic energy of the link mechanism by the energy balance. f_1 is a function for the volume constraint, where c_1 is a positive constant for which there exists $\Omega(\boldsymbol{\phi})$ such that $f_1(\boldsymbol{\phi}) \le 0$.

A shape optimization can be constructed as follows. In the present paper, we assume that the locations of the linkage points $\{\boldsymbol{x}_{\mathrm{J}k}\}_{k \in \mathcal{J}}$ are fixed. Then, the admissible set of domain mappings $\mathcal{C} = \mathcal{C}_1 \times \cdots \times \mathcal{C}_{|\mathcal{L}|}$ in (5) must be replaced by

$$\mathcal{K} = \Big\{ \left(\boldsymbol{\phi}_1, \cdots, \boldsymbol{\phi}_{|\mathcal{L}|}\right)^{\mathrm{T}} \in \mathcal{C} \;\Big|\; \boldsymbol{\phi}_l(\boldsymbol{x}_{\mathrm{J}k}) = \boldsymbol{x}_{\mathrm{J}k},\ k \in \mathcal{J},\ l \in \mathcal{L}, \text{ constraints in design} \Big\}. \tag{44}$$

Problem 3 (Shape optimization problem) Let $\boldsymbol{b}$ and $\boldsymbol{p}$ be given as in Definition 5, and $\boldsymbol{y}_0 = (\boldsymbol{q}_0, \boldsymbol{q}_1, \boldsymbol{0})^{\mathrm{T}}$ be given as in Problem 2. For $\boldsymbol{\phi} \in \mathcal{K}$, let $\boldsymbol{y}$ be the solution of Problem 2, and $f_0(\boldsymbol{\phi}, \boldsymbol{y})$ and $f_1(\boldsymbol{\phi})$ be defined in (42) and (43), respectively. Find $\Omega(\boldsymbol{\phi})$ such that

$$\min_{\boldsymbol{\phi} \in \mathcal{K}} \Big\{ f_0(\boldsymbol{\phi}, \boldsymbol{y}) \;\Big|\; f_1(\boldsymbol{\phi}) \le 0,\ \text{Problem 2},\ \boldsymbol{y} - \bar{\boldsymbol{y}} \in Y \Big\}.$$

5 Shape derivatives of cost functions

To solve Problem 3 by the gradient method, the Fréchet derivatives of the cost functions with respect to the domain variation, which we call the shape derivatives, are required. Let

$$\boldsymbol{\varphi} = \left(\boldsymbol{\varphi}_1, \cdots, \boldsymbol{\varphi}_{|\mathcal{L}|}\right)^{\mathrm{T}} \in V^{|\mathcal{L}|} \tag{45}$$

denote the variation of $\boldsymbol{\phi}$. We refer to the Fréchet derivative of $f_0(\boldsymbol{\phi}, \boldsymbol{y})$ with respect to $\boldsymbol{\varphi}$ as the shape derivative of f_0, denoted as $f_0'(\boldsymbol{\phi}, \boldsymbol{y})[\boldsymbol{\varphi}] = \langle \boldsymbol{g}_0, \boldsymbol{\varphi} \rangle$, where $\langle \cdot, \cdot \rangle$ denotes the dual product. Here, $\boldsymbol{g}_0$ is referred to as the shape gradient for f_0.

Let us derive the equation to compute the shape derivative for f_0. Since Problem 2 is an equality constraint for $f_0(\boldsymbol{\phi}, \boldsymbol{y})$, we can obtain the shape derivative of f_0 by the Lagrange multiplier method. For $\boldsymbol{y} = \left(\boldsymbol{q}^{\mathrm{T}}, \dot{\boldsymbol{q}}^{\mathrm{T}}, \boldsymbol{\eta}^{\mathrm{T}}\right)^{\mathrm{T}}$ such that $\boldsymbol{y} - \bar{\boldsymbol{y}} \in Y$, let

$$\mathscr{L}_0(\boldsymbol{\phi}, \boldsymbol{y}, \boldsymbol{z}_0) = f_0(\boldsymbol{\phi}, \boldsymbol{y}) + \mathscr{L}_{\mathrm{MD}}(\boldsymbol{\phi}, \boldsymbol{y}, \boldsymbol{z}_0) \tag{46}$$

be the Lagrangian for f_0, where $\mathscr{L}_{\mathrm{MD}}(\boldsymbol{\phi}, \boldsymbol{y}, \boldsymbol{z}_0)$ is defined in (41), $\boldsymbol{z}_0$ such that $\boldsymbol{z}_0 - \bar{\boldsymbol{z}}_0 \in Z$ and $\bar{\boldsymbol{z}}_0(t_1) = \boldsymbol{y}(t_1)$ is used as the Lagrange multiplier for f_0. If $\boldsymbol{y}$ is the solution of Problem 2, the stationary condition of $\mathscr{L}_0$ with respect to arbitrary variation $\boldsymbol{z}_0' \in Z$ of $\boldsymbol{z}_0$ such as

$$\begin{aligned}
&\mathscr{L}_{0\boldsymbol{z}_0}(\boldsymbol{\phi}, \boldsymbol{y}, \boldsymbol{z}_0)[\boldsymbol{z}_0'] = \left\langle \frac{\partial \mathscr{L}_0(\boldsymbol{\phi}, \boldsymbol{y}, \boldsymbol{z}_0)}{\partial \boldsymbol{z}_0}, \boldsymbol{z}_0' \right\rangle \\
&= \int_0^{t_1} \Big\{ \Big(-\boldsymbol{M}\ddot{\boldsymbol{q}} - \left(\boldsymbol{\psi}_{\boldsymbol{q}^{\mathrm{T}}}(\boldsymbol{q})\right)^{\mathrm{T}} \dot{\boldsymbol{\eta}} + \boldsymbol{s}(\boldsymbol{\phi}, \boldsymbol{q}, \boldsymbol{b}, \boldsymbol{p}) \Big) \cdot \dot{\boldsymbol{r}}_0' \\
&- \ddot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}}, \ddot{\boldsymbol{q}}] \cdot \boldsymbol{\mu}_0' + \dot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{q}}] \cdot \dot{\boldsymbol{\mu}}_0' \Big\} \mathrm{d}t \\
&= 0
\end{aligned}$$

holds. The stationary condition of $\mathscr{L}_0$ with respect to arbitrary variations $\boldsymbol{y}' = \left(\boldsymbol{q}'^{\mathrm{T}}, \dot{\boldsymbol{q}}'^{\mathrm{T}}, \boldsymbol{\eta}'^{\mathrm{T}}\right)^{\mathrm{T}} \in Y$ of $\boldsymbol{y}$ such as

$$\begin{aligned}
&\mathscr{L}_{0\boldsymbol{y}}(\boldsymbol{\phi}, \boldsymbol{y}, \boldsymbol{z}_0)[\boldsymbol{y}'] \\
&= \int_0^{t_1} \Big\{ \Big(\boldsymbol{M}\ddot{\boldsymbol{r}}_0 + \left(\boldsymbol{\psi}_{\boldsymbol{q}^{\mathrm{T}}}(\boldsymbol{q})\right)^{\mathrm{T}} \dot{\boldsymbol{\mu}}_0 - \boldsymbol{s}(\boldsymbol{\phi}, \boldsymbol{q}, \boldsymbol{b}, \boldsymbol{p}) \Big) \cdot \dot{\boldsymbol{q}}' \\
&+ \ddot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{r}}_0, \ddot{\boldsymbol{r}}_0] \cdot \boldsymbol{\eta}' - \dot{\boldsymbol{\psi}}(\boldsymbol{q})[\dot{\boldsymbol{r}}_0] \cdot \dot{\boldsymbol{\eta}}' \Big\} \mathrm{d}t \\
&= 0
\end{aligned}$$

holds if $\boldsymbol{z}_0 \in Z$ is the solution of the following adjoint problem.

Problem 4 (Adjoint problem for f_0) Let $\boldsymbol{y} = \left(\boldsymbol{q}^{\mathrm{T}}, \dot{\boldsymbol{q}}^{\mathrm{T}}, \boldsymbol{\eta}^{\mathrm{T}}\right)^{\mathrm{T}}$ be the solution of Problem 2. Find $\boldsymbol{z}_0 =$

$\left(\boldsymbol{r}_0^{\mathrm{T}}, \dot{\boldsymbol{r}}_0^{\mathrm{T}}, \boldsymbol{\mu}_0^{\mathrm{T}}\right)^{\mathrm{T}} \in H^1\left((0,t_1);\mathbb{R}^n\right)$, such that

$$\boldsymbol{M}\ddot{\boldsymbol{r}}_0 = \boldsymbol{s}\left(\boldsymbol{b},\boldsymbol{p}\right) \quad \text{in } (0,t_1), \tag{47}$$
$$\ddot{\boldsymbol{\psi}}\left(\boldsymbol{r}_0\right)\left[\dot{\boldsymbol{r}}_0, \ddot{\boldsymbol{r}}_0\right] = \boldsymbol{0} \quad \text{in } (0,t_1), \tag{48}$$
$$\dot{\boldsymbol{\psi}}\left(\boldsymbol{r}_0\right)\left[\dot{\boldsymbol{r}}_0\right] = \boldsymbol{0} \quad \text{in } (0,t_1), \tag{49}$$
$$\dot{\boldsymbol{r}}_0(t_1) = \dot{\boldsymbol{q}}(t_1), \tag{50}$$
$$\boldsymbol{r}_0(t_1) = \boldsymbol{q}(t_1). \tag{51}$$

The variational form of Problem 4 can be written as follows.

Problem 5 (Variational form of Problem 4) Let $\boldsymbol{y} = \left(\boldsymbol{q}^{\mathrm{T}}, \dot{\boldsymbol{q}}^{\mathrm{T}}, \boldsymbol{\eta}^{\mathrm{T}}\right)^{\mathrm{T}}$ be the solution of Problem 2. Find $\boldsymbol{z}_0 = \left(\boldsymbol{r}_0^{\mathrm{T}}, \dot{\boldsymbol{r}}_0^{\mathrm{T}}, \boldsymbol{\mu}_0^{\mathrm{T}}\right)^{\mathrm{T}}$ such that $\boldsymbol{z}_0 - \bar{\boldsymbol{z}} \in Z$, satisfying

$$\begin{aligned}\mathscr{L}_{0\boldsymbol{y}}\left(\boldsymbol{\phi},\boldsymbol{y},\boldsymbol{z}_0\right)\left[\boldsymbol{y}'\right] = \int_0^{t_1} \Big\{ \Big(\boldsymbol{A}\left(\boldsymbol{\phi},\boldsymbol{q}\right)\dot{\boldsymbol{z}}_0 + \boldsymbol{B}\left(\boldsymbol{\phi}\right)\boldsymbol{z}_0 \\ - \boldsymbol{h}\left(\boldsymbol{\phi},\boldsymbol{q},\boldsymbol{b},\boldsymbol{p}\right)\Big)\cdot\boldsymbol{y}' - \dot{\boldsymbol{\psi}}\left(\boldsymbol{q}\right)\left[\dot{\boldsymbol{r}}_0\right]\cdot\boldsymbol{\eta}' \Big\}\,\mathrm{d}t \\ = 0\end{aligned}$$

for all $\boldsymbol{y}' = \left(\boldsymbol{q}'^{\mathrm{T}}, \dot{\boldsymbol{q}}'^{\mathrm{T}}, \boldsymbol{\eta}'^{\mathrm{T}}\right)^{\mathrm{T}} \in Y$, where $\bar{\boldsymbol{z}}$ is an arbitrary function satisfying $\bar{\boldsymbol{z}}(t_1) = \boldsymbol{y}(t_1)$, and Y and Z are the same as in Problem 2.

Then, we have the ordinary differential equation from Problem 5 as

$$\boldsymbol{A}\left(\boldsymbol{\phi},\boldsymbol{q}\right)\dot{\boldsymbol{z}}_0 + \boldsymbol{B}\left(\boldsymbol{\phi}\right)\boldsymbol{z}_0 = \boldsymbol{h}\left(\boldsymbol{\phi},\boldsymbol{q},\boldsymbol{b},\boldsymbol{p}\right).$$

This equation system can be solved by the same numerical integration scheme as the problem 2. However, using the terminal condition (35), time goes back from $t = t_1$ to 0.

Moreover, in the case that $\boldsymbol{y} = \left(\boldsymbol{q}^{\mathrm{T}}, \dot{\boldsymbol{q}}^{\mathrm{T}}, \boldsymbol{\eta}^{\mathrm{T}}\right)^{\mathrm{T}}$ and $\boldsymbol{z}_0 = \left(\boldsymbol{r}_0^{\mathrm{T}}, \dot{\boldsymbol{r}}_0^{\mathrm{T}}, \boldsymbol{\mu}_0^{\mathrm{T}}\right)^{\mathrm{T}}$ are fixed at the solutions of Problems 2 and 5, respectively, by applying the formulae of shape derivatives for domain and boundary integrals [10] to $\mathscr{L}_0$ defined in (46), we have

$$\begin{aligned}&f_0'\left(\boldsymbol{\phi},\boldsymbol{y}\right)\left[\boldsymbol{\varphi}\right] = \mathscr{L}_{0\boldsymbol{\phi}}\left(\boldsymbol{\phi},\boldsymbol{y},\boldsymbol{z}_0\right)\left[\boldsymbol{\varphi}\right] \\ &= \sum_{l\in\mathcal{L}}\Bigg\{\int_{\partial\Omega_l(\boldsymbol{\phi}_l)}\Big(g_{\boldsymbol{b}0l}\left(\boldsymbol{q}_l,\boldsymbol{r}_l\right) + g_{\boldsymbol{M}0l}\left(\boldsymbol{q}_l,\boldsymbol{r}_l\right)\Big)\boldsymbol{\nu}\cdot\boldsymbol{\varphi}\,\mathrm{d}\gamma \\ &+ \int_{\partial\Omega_l(\boldsymbol{\phi}_l)\cap\Gamma_{pl}(\boldsymbol{\phi}_l)} g_{p0l}\left(\boldsymbol{q}_l,\boldsymbol{r}_l\right)\boldsymbol{\nu}\cdot\boldsymbol{\varphi}\,\mathrm{d}\gamma\Bigg\} \\ &= \sum_{l\in\mathcal{L}}\int_{\partial\Omega_l(\boldsymbol{\phi}_l)} g_{0l}\left(\boldsymbol{q}_l,\boldsymbol{r}_l\right)\boldsymbol{\nu}\cdot\boldsymbol{\varphi}\,\mathrm{d}\gamma \\ &= \sum_{l\in\mathcal{L}}\left\langle g_{0l}\left(\boldsymbol{q}_l,\boldsymbol{r}_l\right)\boldsymbol{\nu},\boldsymbol{\varphi}\right\rangle\end{aligned} \tag{52}$$

for all domain variations $\boldsymbol{\varphi}$, where

$$g_{\boldsymbol{b}0l}\left(\boldsymbol{q}_l,\boldsymbol{r}_l\right) = \int_0^{t_1} \boldsymbol{b}_l\cdot\boldsymbol{u}_l\left(\dot{\boldsymbol{r}}_l - \dot{\boldsymbol{q}}_l\right)\,\mathrm{d}t, \tag{53}$$

$$g_{\boldsymbol{M}0l}\left(\boldsymbol{q}_l,\boldsymbol{r}_l\right) = -\int_0^{t_1} \rho_l\boldsymbol{u}_l\left(\ddot{\boldsymbol{q}}_l\right)\cdot\boldsymbol{u}_l\left(\dot{\boldsymbol{r}}_l\right)\,\mathrm{d}t, \tag{54}$$

$$g_{p0l}\left(\boldsymbol{q}_l,\boldsymbol{r}_l\right) = \int_0^{t_1} \left(\kappa + \partial_\nu\right)\left(\boldsymbol{p}_l\cdot\boldsymbol{u}_l\left(\dot{\boldsymbol{r}}_l - \dot{\boldsymbol{q}}_l\right)\right)\,\mathrm{d}t, \tag{55}$$

where $\kappa = \boldsymbol{\nabla}\cdot\boldsymbol{\nu}$ is the curvature, and $\partial_\nu = \boldsymbol{\nu}\cdot\boldsymbol{\nabla}$. Here, $g_{0l}\left(\boldsymbol{q}_l,\boldsymbol{r}_l\right)\boldsymbol{\nu}$ belongs to the piecewise C^0 class.

On the other hand, the shape derivative of $f_1\left(\boldsymbol{\phi}\right)$ with respect to $\boldsymbol{\varphi}$ is obtained as

$$\begin{aligned}f_1'\left(\boldsymbol{\phi}\right)\left[\boldsymbol{\varphi}\right] &= \sum_{l\in\mathcal{L}}\int_{\partial\Omega_l(\boldsymbol{\phi}_l)} -\boldsymbol{\nu}\cdot\boldsymbol{\varphi}\,\mathrm{d}\gamma \\ &= \sum_{l\in\mathcal{L}}\int_{\partial\Omega_l(\boldsymbol{\phi}_l)} g_{1l}\boldsymbol{\nu}\cdot\boldsymbol{\varphi}\,\mathrm{d}\gamma = \sum_{l\in\mathcal{L}}\left\langle g_{1l}\boldsymbol{\nu},\boldsymbol{\varphi}\right\rangle.\end{aligned} \tag{56}$$

Here, $g_{1l}\boldsymbol{\nu} = -\boldsymbol{\nu}$ belongs to the piecewise C^0 class.

6 The $\boldsymbol{H^1}$ gradient method

The H^1 gradient method is proposed as a method for finding the variation of the design variable, such as the domain mapping or the density parameter that decreases a cost function, as a solution to a boundary value problem of an elliptic partial differential equation[6,5,4]. In the case that a shape derivative $\boldsymbol{g}_{il}$ of a cost function $f_i\left(\boldsymbol{\phi}\right)$ for $i\in\{0,1\}$ and the $l\in\mathcal{L}$-th link is given, the H^1 gradient method can be described as follows (Fig. 4).

Problem 6 (H^1 gradient method) Let X be a Hilbert space of $H^1\left(D_0;\mathbb{R}^d\right)$, and let $b: X\times X\to\mathbb{R}$ be a coercive bilinear form on X such that there exists $\alpha > 0$ that satisfies

$$a\left(\boldsymbol{w},\boldsymbol{w}\right) \geq \alpha\left\|\boldsymbol{w}\right\|_X^2$$

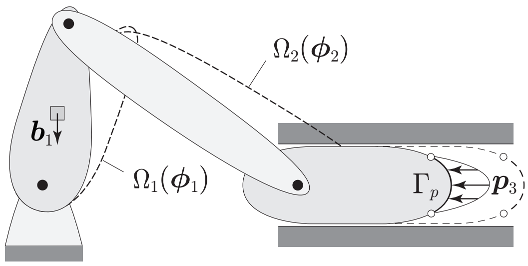
for all $\boldsymbol{w}\in X$. For $\boldsymbol{g}_{il}\in X'$ (dual space of X), which is a Fréchet derivative of cost function $f\left(\boldsymbol{\phi}\right)$ at $\boldsymbol{\phi}\in X$, find $\boldsymbol{\varphi}_{gil}\in X$ such that

$$a\left(\boldsymbol{\varphi}_{gil},\boldsymbol{w}\right) = -\left\langle\boldsymbol{g}_{il},\boldsymbol{w}\right\rangle \tag{57}$$

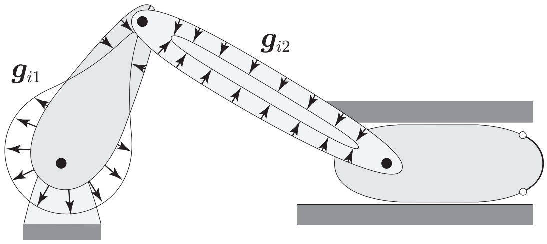
for all $\boldsymbol{w}\in X$.

The existence of a unique solution of Problem 6 is shown by the Lax-Milgram theorem. We can confirm that the solutions

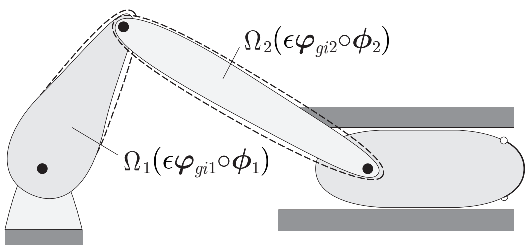
$$\boldsymbol{\varphi}_{gi} = \left(\boldsymbol{\varphi}_{gi1},\cdots,\boldsymbol{\varphi}_{gi|\mathcal{L}|}\right)^{\mathrm{T}} \in V^{|\mathcal{L}|}$$



(a) Main / Adjoint problem (DAE)



(b) H^1 gradient method



(c) Reshaping

Fig. 4 H^1 gradient method for reshaping to decrease f_i

of the H^1 gradient method decrease f_i as

$$
\begin{aligned}
&f_i\left(\boldsymbol{\phi}+\boldsymbol{\varphi}_{gi}\right)-f_i\left(\boldsymbol{\phi}\right)=\sum_{l\in\mathcal{L}}\left(\left\langle \boldsymbol{g}_{il},\boldsymbol{\varphi}_{gil}\right\rangle+o\left(\left\|\boldsymbol{\varphi}_{gil}\right\|_X\right)\right)\\
&=\sum_{l\in\mathcal{L}}\left(-\left\langle \boldsymbol{\varphi}_{gil},\boldsymbol{\varphi}_{gil}\right\rangle+o\left(\left\|\boldsymbol{\varphi}_{gil}\right\|_X\right)\right)\\
&\le\sum_{l\in\mathcal{L}}\left(-\alpha\left\|\boldsymbol{\varphi}_{gil}\right\|_X^2+o\left(\left\|\boldsymbol{\varphi}_{gil}\right\|_X\right)\right).
\end{aligned}
$$

Moreover, we can consider that $\boldsymbol{\varphi}_{gi}$ can belong to $\mathcal{C}$ and $\mathcal{K}$ as follows. Since $\partial\Omega\left(\boldsymbol{\phi}\right)$ is the piecewise C^1 class, $\boldsymbol{\nu}$ is the piecewise C^0 class. Also, since Γ_{p0} is the piecewise C^2 class, κ is the C^0 class. Then, $\boldsymbol{g}_{0l}=g_{0l}\boldsymbol{\nu}$ in (52) and $\boldsymbol{g}_{1l}=-\boldsymbol{\nu}$ in (56) belong to the piecewise C^0 class that is included in X'. On the other hand, the solutions $\boldsymbol{\varphi}_{gil}$ of Problem 6 improves one-time differentiability on boundary. Then, it is expected that the $\boldsymbol{\varphi}_{gil}$ have the piecewise C^1 class on $\partial\Omega\left(\boldsymbol{\phi}\right)$. If Γ_{p0} is fixed in Problem 3, i.e., $\boldsymbol{\phi}\left(\Gamma_{p0}\right)=\Gamma_{p0}$ is added in the constraint of $\mathcal{K}$ in (44), the piecewise C^1 class of $\boldsymbol{\varphi}_{gil}$ is enough that $\boldsymbol{\varphi}_{gil}\circ\boldsymbol{\phi}_{il}$ for all $l\in\mathcal{L}$ belong to $\mathcal{C}$ and $\mathcal{K}$. Here, $\circ$ denotes a composite function as $\boldsymbol{\varphi}_{gil}\circ\boldsymbol{\phi}_{il}=\boldsymbol{\varphi}_{gil}\left(\boldsymbol{\phi}_{il}\right)$.

In the case that Γ_{p0} is allowed to vary, some additional smoothing treatment may be required in order that the varied domains $\boldsymbol{\varphi}_{gil}\circ\boldsymbol{\phi}_{il}$ for all $l\in\mathcal{L}$ remain in $\mathcal{C}$ and $\mathcal{K}$.

For the coercive bilinear form $a\left(\,\cdot\,,\,\cdot\,\right)$ in Problem 6, we use

$$
\begin{aligned}
&a\left(\boldsymbol{\varphi}_{gil},\boldsymbol{w}\right)=c_a\int_{\Omega(\boldsymbol{\phi})}\boldsymbol{E}\left(\boldsymbol{\varphi}_{gil}\right)\cdot\boldsymbol{E}\left(\boldsymbol{w}\right)\mathrm{d}x\\
&+\int_{\Gamma_{0l}}\left\{\boldsymbol{\varphi}_{gil}\cdot\boldsymbol{E}\left(\boldsymbol{w}\right)\boldsymbol{\nu}+\boldsymbol{w}\cdot\boldsymbol{E}\left(\boldsymbol{\varphi}_{gil}\right)\boldsymbol{\nu}\right\}\mathrm{d}\gamma \qquad (58)
\end{aligned}
$$

for the $l\in\mathcal{L}$-th link. Here,

$$
\boldsymbol{E}\left(\boldsymbol{w}\right)=\frac{1}{2}\left(\boldsymbol{\nabla}\boldsymbol{w}^{\mathrm{T}}+\left(\boldsymbol{\nabla}\boldsymbol{w}^{\mathrm{T}}\right)^{\mathrm{T}}\right)
$$

are the linear strain. Γ_{0l}, such that $\left|\Gamma_{0l}\right|>0$, is a prescribed boundary on which the domain variation is fixed. If the $l\in\mathcal{L}$-th link has linkage conditions, then the boundaries of the neighborhoods of the linkage points must be included in Γ_{0l}. The boundaries related to the constraints in the design defined in (44) must also be included in Γ_{0l}. Moreover, c_a is a positive constant for controlling the magnitude of $\boldsymbol{\varphi}_{gil}$ in Problem 6.

Using $a\left(\,\cdot\,,\,\cdot\,\right)$ of (58), the strong form of Problem 6 can be written as follows.

Problem 7 (H^1 gradient method) Let $\boldsymbol{g}_{il}\in X'$ be given. Find $\boldsymbol{\varphi}_{gil}\in X$ such that

$$
\begin{aligned}
&-\boldsymbol{\nabla}^{\mathrm{T}}\boldsymbol{E}\left(\boldsymbol{\varphi}_{gil}\right)=\boldsymbol{0}^{\mathrm{T}}\quad \text{in } \Omega_l\left(\boldsymbol{\phi}_l\right),\\
&\boldsymbol{E}\left(\boldsymbol{\varphi}_{gil}\right)\boldsymbol{\nu}=-\boldsymbol{g}_{il}\quad \text{on } \partial\Omega_l\left(\boldsymbol{\phi}_l\right)\setminus\Gamma_{0l}\\
&\boldsymbol{\varphi}_{gil}=\boldsymbol{0}\quad \text{on } \Gamma_{0l}.
\end{aligned}
$$

Although X is defined as a set of functions defined in D_0, Problem 7 is a boundary value problem of an elliptic partial differential equation in $\Omega_l\left(\boldsymbol{\phi}_l\right)$. The existence of an extension operator from a function $\boldsymbol{\varphi}_{gil}$ in $H^1\left(\Omega_l\left(\boldsymbol{\phi}_l\right);\mathbb{R}^d\right)$ into $H^1\left(D_0;\mathbb{R}^d\right)$ is shown by Calderon's extension theorem[1].

If we use the Cauchy stress

$$
\boldsymbol{S}\left(\boldsymbol{w}\right)=\boldsymbol{C}\boldsymbol{E}\left(\boldsymbol{w}\right),
$$

instead of $\boldsymbol{E}\left(\boldsymbol{w}\right)$ in Problem 7, where

$$
\boldsymbol{C}:D_0\to\mathbb{R}^{d\times d\times d\times d}
$$

is an elliptic and bounded function denoting the stiffness of the linear elastic continuum, i.e., there exists $\alpha,\beta>0$ such that

$$
\boldsymbol{\xi}\cdot\boldsymbol{C}\boldsymbol{\xi}\ge\alpha\left\|\boldsymbol{\xi}\right\|^2,\quad \left|\boldsymbol{\xi}\cdot\boldsymbol{C}\boldsymbol{\eta}\right|\le\beta\left\|\boldsymbol{\xi}\right\|\left\|\boldsymbol{\eta}\right\|
$$

for all $\boldsymbol{\xi}, \boldsymbol{\eta} \in \left\{ \boldsymbol{\xi} \in \mathbb{R}^{d \times d} \mid \boldsymbol{\xi} = \boldsymbol{\xi}^{\mathrm{T}} \right\}$ in D_0. Then, Problem 7 using $\boldsymbol{S}(\boldsymbol{w})$ instead of $\boldsymbol{E}(\boldsymbol{w})$ agrees with a linear elastic problem defined in $\Omega_l(\boldsymbol{\phi}_l)$ loaded with a fictitious traction of $-\boldsymbol{g}_{il}$ on the boundary $\partial\Omega_l(\boldsymbol{\phi}_l) \setminus \Gamma_{0l}$.

The Problem 7 or the corresponding linear elastic problem can be solved by the standard finite element method. The use of the H^1 gradient method to solve Problem 3 is described in the next section.

7 Solution to the shape optimization problem

We use the following iterative method based on sequential quadratic programming to solve Problem 3. To determine the domain variation decreasing $f_0(\boldsymbol{\phi}, \boldsymbol{y})$ while satisfying $f_1(\boldsymbol{\phi}) \leq 0$, let us consider the following problem. In this section, we use the notation $f_0(\boldsymbol{\phi}, \boldsymbol{y}) = f_0(\boldsymbol{\phi})$.

Problem 8 (SQ approximation) For $\boldsymbol{\phi} \in \mathcal{K}$, let $\boldsymbol{g}_{il}$ be the shape derivatives of f_i for $i \in \{0,1\}$ and the $l \in \mathcal{L}$-th link, and let $f_1(\boldsymbol{\phi}) \leq 0$. Let $a(\cdot, \cdot)$ be given as in (58). Find $\boldsymbol{\varphi} = \left(\boldsymbol{\varphi}_1, \cdots, \boldsymbol{\varphi}_{|\mathcal{L}|}\right)^{\mathrm{T}}$ such that

$$\min_{\boldsymbol{\varphi} \in V^{|\mathcal{L}|}} \left\{ q(\boldsymbol{\varphi}) = \sum_{l \in \mathcal{L}} \left(\frac{1}{2} a(\boldsymbol{\varphi}_l, \boldsymbol{\varphi}_l) + \langle \boldsymbol{g}_{0l}, \boldsymbol{\varphi}_l \rangle \right) \;\middle|\; f_1(\boldsymbol{\phi}) + \sum_{l \in \mathcal{L}} \left(\langle \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_l \rangle \right) \leq 0 \right\}.$$

The Lagrangian of Problem 8 is defined as

$$\mathscr{L}_{\mathrm{SQ}}(\boldsymbol{\varphi}, \lambda_1) = q(\boldsymbol{\varphi}) + \lambda_1 \cdot \left(f_1(\boldsymbol{\phi}) + \sum_{l \in \mathcal{L}} \langle \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_l \rangle \right)$$

where $\lambda_1 \in \mathbb{R}$ is the Lagrange multiplier for the constraint $f_1(\boldsymbol{\varphi}) \leq 0$. The Karush–Kuhn–Tucker conditions for Problem 8 are given as

$$a(\boldsymbol{\varphi}_l, \boldsymbol{\varphi}_l) + \langle \boldsymbol{g}_{0l} + \lambda_1 \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_l \rangle = 0, \text{ for } l \in \mathcal{L} \tag{59}$$

$$f_1(\boldsymbol{\phi}) + \sum_{l \in \mathcal{L}} \langle \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_l \rangle \leq 0, \tag{60}$$

$$\lambda_1 \left(f_1(\boldsymbol{\phi}) + \sum_{l \in \mathcal{L}} \langle \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_l \rangle \right) = 0, \tag{61}$$

$$\lambda_1 \geq 0 \tag{62}$$

for all $\boldsymbol{\varphi} \in V^{|\mathcal{L}|}$.

Here, let $\boldsymbol{\varphi}_{gil}$ for $i \in \{0,1\}$ and $l \in \mathcal{L}$ be the solutions to Problem 6, and set

$$\boldsymbol{\varphi}_{gl} = \boldsymbol{\varphi}_{g0l} + \lambda_1 \boldsymbol{\varphi}_{g1l}, \tag{63}$$

$$\boldsymbol{\varphi}_g = \left(\boldsymbol{\varphi}_{g1}, \cdots, \boldsymbol{\varphi}_{g|\mathcal{L}|}\right)^{\mathrm{T}}. \tag{64}$$

Then, by substituting $\boldsymbol{\varphi}_{gl}$ of (63) for $\boldsymbol{\varphi}_l$ in (59), (59) holds. If the constraint in (60) is active, i.e., (60) holds with the equality, we have

$$\sum_{l \in \mathcal{L}} \langle \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_{g1l} \rangle \lambda_1 = -f_1(\boldsymbol{\phi}) + \sum_{l \in \mathcal{L}} \langle \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_{g0l} \rangle. \tag{65}$$

Equation (65) has a unique solution of λ_1. Moreover, if $f_1(\boldsymbol{\phi}) = 0$, we have

$$\sum_{l \in \mathcal{L}} \langle \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_{g1l} \rangle \lambda_1 = -\sum_{l \in \mathcal{L}} \langle \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_{g0l} \rangle. \tag{66}$$

Since (66) is independent of the magnitude of $\boldsymbol{\varphi}_{g0l}$ and $\boldsymbol{\varphi}_{g1l}$ for all $l \in \mathcal{L}$, (66) is used in the algorithm shown later for the initial domain Ω_0 in which we assume $f_1(\boldsymbol{\phi}) \leq 0$ is satisfied. If $\lambda_1 < 0$ in the solution λ_1 to (65) or (66), by putting $\lambda_1 = 0$, we have λ_1 satisfying (59) to (62).

The step size for domain variation should be given by using the norm of $\boldsymbol{\varphi}_g \in V$. In the present paper, we use

$$|\boldsymbol{\varphi}_g|_{V_\Omega} = \operatorname*{ess\,sup}_{\boldsymbol{x} \in \Omega_l(\boldsymbol{\phi}_l),\ l \in \mathcal{L}} \left\{ |E_{ij}(\boldsymbol{\varphi}_{gl})|,\ i, j \in \{1, \cdots, d\} \right\}$$

as a measure for the step size for domain variation. It is adjusted by the selection of c_a in (58) using criteria such as Armijo's and Wolfe's criteria[3,11] ensuring the Zoutendijk condition for global convergence in the original shape optimization problem[9]. Let

$$\mathscr{L}(\boldsymbol{\phi}, \boldsymbol{\eta}) = f_0(\boldsymbol{\phi}) + \lambda_1 f_1(\boldsymbol{\phi})$$

be the Lagrangian for the original optimization problem, and let λ_1 satisfy (60) through (62). A criterion for the maximum limit of $|\boldsymbol{\varphi}_g|_{V_\Omega}$ is given by Armijo's criterion as

$$\mathscr{L}(\boldsymbol{\varphi}_g \circ \boldsymbol{\phi}, \lambda_1) - \mathscr{L}(\boldsymbol{\phi}, \lambda_1) \leq \xi \sum_{l \in \mathcal{L}} \langle \boldsymbol{g}_{0l} + \lambda_1 \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_{gl} \rangle \tag{67}$$

for a constant $\xi \in (0,1)$, where

$$\boldsymbol{\varphi}_g \circ \boldsymbol{\phi} = \left(\boldsymbol{\varphi}_{g1} \circ \boldsymbol{\phi}_1, \cdots, \boldsymbol{\varphi}_{g|\mathcal{L}|} \circ \boldsymbol{\phi}_{|\mathcal{L}|}\right)^{\mathrm{T}}.$$

The minimum limit of $|\boldsymbol{\varphi}_g|_{V_\Omega}$ is given by Wolfe's criterion as

$$\mu \sum_{l \in \mathcal{L}} \langle \boldsymbol{g}_{0l} + \lambda_1 \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_{gl} \rangle \leq \sum_{l \in \mathcal{L}} \langle \boldsymbol{g}_{0l\,\mathrm{new}} + \lambda_{1\,\mathrm{new}} \boldsymbol{g}_{1l\,\mathrm{new}}, \boldsymbol{\varphi}_{gl} \rangle \tag{68}$$

using a constant μ such that $0 < \xi < \mu < 1$, where $(\cdot)_{\mathrm{new}}$ means the function at $\boldsymbol{\varphi}_{gl} \circ \boldsymbol{\phi}_l$ for $l \in \mathcal{L}$.

In order to ensure that $f_1(\boldsymbol{\varphi}_g \circ \boldsymbol{\phi}) \leq 0$ is satisfied, we add a routine updating λ_1 by $\lambda_{1\,\mathrm{new}} = \lambda_1 + \delta\lambda_1$, where $\delta\lambda_1$ is determined by

$$\sum_{l\in\mathcal{L}} \langle \boldsymbol{g}_{1l}, \boldsymbol{\varphi}_{g1l} \rangle \, \delta\lambda_1 = -f_1(\boldsymbol{\varphi}_g \circ \boldsymbol{\phi}), \tag{69}$$

where $\boldsymbol{\varphi}_g$ is of in (64) using old λ_1.

Combining the above considerations, we propose the following numerical scheme. Let $f_1(\boldsymbol{\phi}) \leq 0$ be satisfied for Ω_0.

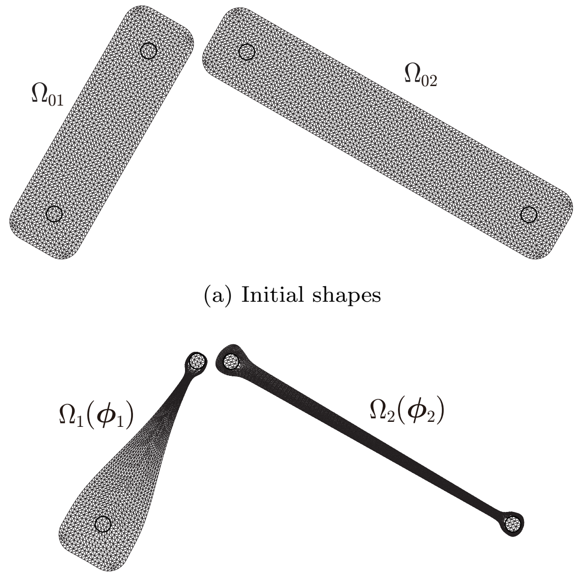
(i) Set $\Omega_0 = \{\Omega_{01}, \cdots, \Omega_{0|\mathcal{L}|}\}$, c_a in (58), initial step size $\epsilon > 0$ for $|\boldsymbol{\varphi}_g|_{V_\Omega}$, ex. $\epsilon = 0.01$, parameters of Armijo's and Wolfe's criteria ξ and μ such that $0 < \xi < \mu < 1$, convergence rate $\epsilon_0 > 0$ for $|\boldsymbol{\varphi}_g|_{V_\Omega}$, ex. $\epsilon_0 = 0.001$, and $k = 0$.
(ii) Compute f_i and $\boldsymbol{g}_{il}$ for $i \in \{0, 1\}$ and $l \in \mathcal{L}$ at Ω_0.
(iii) Solve $\boldsymbol{\varphi}_{gil}$ for $i \in \{0, 1\}$ and $l \in \mathcal{L}$ in Problem 6.
(iv) Solve λ_1 as follows.
  – If $f_1 < 0$, set $\lambda_1 = 0$ and proceed to the next step.
  – Otherwise, compute λ_1 by (66) at $k = 0$ or (65) at $k > 0$.
  – If $\lambda_1 \geq 0$ is satisfied, proceed to the next step. Otherwise, set $\lambda_1 = 0$.
(v) Calculate $\boldsymbol{\varphi}_g$ by (64). If $k = 0$, modify c_a such that $|\boldsymbol{\varphi}_g|_{V_\Omega} = \epsilon$. Compute f_i for $i \in \{0, 1\}$ at

$$\Omega(\boldsymbol{\varphi}_g \circ \boldsymbol{\phi}) = \{\Omega_1(\boldsymbol{\varphi}_{g1} \circ \boldsymbol{\phi}_1), \cdots, \Omega_{|\mathcal{L}|}(\boldsymbol{\varphi}_{g|\mathcal{L}|} \circ \boldsymbol{\phi}_{|\mathcal{L}|})\}.$$

  – If $f_1(\boldsymbol{\varphi}_g \circ \boldsymbol{\phi}) \leq 0$, proceed to the next step.
  – Otherwise, do the following. Set λ_{10} by λ_1, and $j = 0$. (∗) Solve (69) for $\delta\lambda_1$. Set $\lambda_1 = \lambda_{1\,j+1}$ by $\lambda_{1j} + \delta\lambda_1$. If $f_1(\boldsymbol{\varphi}_g \circ \boldsymbol{\phi}) \leq 0$ is not satisfied, set j with $j + 1$, and return to (∗).
(vi) Compute $\boldsymbol{g}_{il}$ for $i \in \{0, 1\}$ and $l \in \mathcal{L}$ at $\Omega(\boldsymbol{\varphi}_g \circ \boldsymbol{\phi})$.
  – If (67) and (68) hold, proceed to the next step.
  – If (67) or (68) does not hold, update c_a with a larger or smaller value. Return to (v).
(vii) Let $\boldsymbol{\phi}_{k+1} = \boldsymbol{\varphi}_g \circ \boldsymbol{\phi}_k$, $\Omega_{k+1} = \Omega(\boldsymbol{\phi}_{k+1})$, and $\lambda_{1k} = \lambda_1$, and judge the terminal condition by $|\boldsymbol{\varphi}_g|_{V_\Omega} \leq \epsilon_0$.
  – If the condition holds, terminate the algorithm.
  – Otherwise, replace $k + 1$ with k and return to (iii).

8 Numerical example

We developed a program for the shape optimization problem of a link mechanism based on the above numerical scheme. Using this program, we analyzed a shape optimization problem of a piston-crank mechanism. Ω_{01} and Ω_{02} in Fig. 1 were chosen as the variable domains.



(a) Initial shapes

(b) Optimum shapes

Fig. 5 Numerical result of shapes with finite element meshes

A constant and left-pointing external force was applied to $\boldsymbol{x}_{\mathrm{J}3}$ in Fig. 2 (a). The terminal time t_1 was decided such that $\theta_1(t_1)$ becomes 13° for the initial shapes. The density $\rho_1 = \rho_2$ was assumed to be constant. c_1 in (43) was set to half of $|\Omega_{01}| + |\Omega_{02}|$. Figure 5 shows the initial and optimum shapes of the two links. The circles in Fig. 5 (a) denote Γ_{0l} in (58). The iteration histories of the cost functions are shown in Fig. 6. In this figure, $f_{0\,\mathrm{init}}$ denotes the value of f_0 in the initial shapes. Since f_0 has a negative value, the iteration histories of the cost functions show that the object function f_0 decreases monotonically and converges while the volume constraint of f_1 is satisfied.

We can observe that material moved so that mobility of the link mechanism is improved. Since we did not use any constraint with respect to elastic deformation or stress, the optimized shapes have less strength. Moreover, dynamic balance is not considered. A shape optimization problem of a link mechanism using cost functions for elastic deformation and dynamic balance still remains to be solved.

9 Conclusions

In the present paper, a shape optimization problem for a link mechanism was formulated using external work done by a given external force, which agrees with the kinetic energy of the link mechanism, for an assigned time interval as the objective function to maximize and the volume of all the links as a constraint function. The evaluation methods for the shape derivatives of

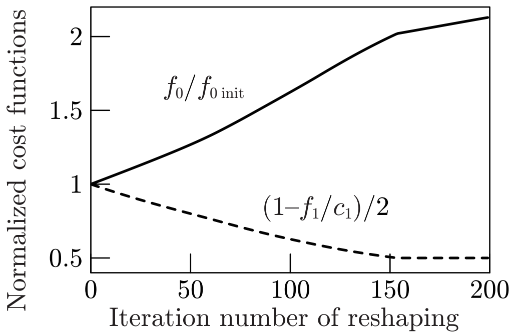


Fig. 6 Iteration history of cost functions with respect to reshapings

these cost functions were presented theoretically. Using the shape derivatives, the H^1 gradient method was employed to obtain the domain variations that decrease the cost functions. A scheme to solve the shape optimization problem with constraints was presented in accordance with sequential quadratic programming. Finally, we illustrated that reasonable shapes of links were obtained by the present approach.

Acknowledgements The present study was supported by JSPS KAKENHI (20540113).

References

1. Adams, R.A., Fournier, J.J.F.: Sobolev spaces, 2nd ed. Academic Press (2003)
2. Amirouche, F.: Fundamentals of multibody dynamics : theory and applications. Birkhäuser, Boston (2006)
3. Armijo, L.: Minimization of functions having lipschitz-continuous first partial derivatives. Pacific J. Math. **16**, 1–3 (1966)
4. Azegami, H., Fukumoto, S., Aoyama, T.: Shape optimization of continua using nurbs as basis functions. Structural and Multidisciplinary Optimization **47**(2), 247–258 (2013)
5. Azegami, H., Kaizu, S., Takeuchi, K.: Regular solution to topology optimization problems of continua. JSIAM Letters **3**, 1–4 (2011)
6. Azegami, H., Takeuchi, K.: A smoothing method for shape optimization: traction method using the Robin condition. International Journal of Computational Methods **3**(1), 21–33 (2006)
7. Bremer, H.: Elastic multibody dynamics : a direct Ritz approach. Springer (2008)
8. Featherstone, R.: Rigid body dynamics algorithms. Springer, New York (2008)
9. Nocedal, J., Wright, S.J.: Numerical optimization. Springer, New York (2006)
10. Sokolowski, J., Zolésio, J.P.: Introduction to Shape Optimization: Shape Sensitivity Analysis. Springer-Verlag, New York (1992)
11. Wolfe, P.: Convergence conditions for ascent methods. SIAM Review **11**, 226–235 (1969)