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Direct Transcription Approach to Dynamic Optimization Problems in Engineering

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Abstract. The direct transcription method that employs global collocation at Legendre-Gauss-Radau points is addressed and applied to infinite-dimensional dynamic optimization problems in engineering. The formulation of these latter is considered referring to a Bolza-type performance index. A reduced unconstrained form of it is particularly studied in the pseudospectral domain and the continuous-to-discrete conversion is thoroughly discussed. An equivalent finite-dimension nonlinear programming problem is therefore obtained and hints on its numerical implementation are given. Eventually, a few benchmark historical problems in engineering are revisited, stated, numerically solved and compared to literature.

Keywords: Direct methods, Continuous dynamic optimization, Orthogonal collocation method, Nonlinear programming.

1. Introduction

Dynamic optimization is a branch of optimization theory which aims to determine the inputs, also called decision (or control) functions, to a dynamical system such that a goal functional (also called a performance index) is minimized or maximized, while satisfying certain constraints on the evolution of the system. It is appreciated that, unlike static optimization problems, inputs are not merely static parameters represented by points in an n -dimensional space but, instead, are functions of the variable along which the system evolves. Consequently, the object to minimize (or maximize) is not a function from \mathbb{R}^n to \mathbb{R} but a functional defined on the infinite-dimensional set of all the possible input functions.

Because of their complexity, situations in which solutions to the dynamic optimization problems are solved in closed form are rarely encountered, hindering one to resort to numerical methods. According to [1], these latter are classified into two main groups: indirect and direct methods. While researchers majorly interested in differential equation theory focus on indirect methods, direct methods have largely been (and are currently being) adopted in optimization techniques.

In indirect methods, principles of calculus of variations are used to derive first-order optimality conditions, leading to a boundary value problem. The optimal solution is then found by solving a system of first-order differential equations that satisfy endpoint conditions. The most well-known strategy pertaining to this approach is the so-called shooting method [2]. However, despite of its simplicity, the shooting method may present significant shortcomings since errors in the unknown boundary conditions may be considerably amplified by the integration process. A solution to this numerical issue is offered by the so-called multiple-shooting methods, where the interval in which integration takes place is divided into many subintervals with initial values of the interior points need to be determined being unknown. Nevertheless, even this latter may not be much helpful if initial guesses are not well prescribed [3].

On the other hand, direct methods have been gaining much interest and their theoretical development is more and more refined leading, together with the increasing improvement of computers generation, to efficient algorithms which numerically solve dynamic optimization problems [4]. Among these methods the so-called direct orthogonal collocation method (or pseudospectral method) has been increasing in popularity. This method permits, as described in details in the following sections, the parameterization of the states and of the control inputs using specified functional forms and collocation is performed at chosen points. In particular, the state (and sometimes the control) variables of the original problem are approximated using global polynomials. The differential equations are then collocated using nodes obtained from quadrature points so that the dynamic optimization problem is transcribed to a standard nonlinear programming (NLP) problem. Due to the exponential convergence, in the most of applications a relatively coarse computational grid suffices to achieve a rather good accuracy.

Several direct transcription methods have been employed considering different types of collocation point sets and polynomial approximation basis functions. As far as collocation points are concerned, a considerable amount of work has been developed by using Chebyshev, Legendre-Gauss (LG), Legendre-Gauss-Lobatto (LGL), Legendre-Gauss-Radau (LGR) and flipped Legendre-Gauss-Radau (f-LGR) points, e.g., [4-8]. A numerical framework for the numerical solution of optimal control problems using most of the aforementioned points is given in [9] with particular attention devoted to the co-state evaluation. On the other hand, as far as the



approximation of the state and of the control is concerned, many attempts have been made available employing Chebyshev [10], Bernstein [11] and, more frequently, Lagrange polynomials [12-14], as these latter satisfy the isolation property (see Section 2, below).

Notwithstanding a considerable amount of work dealing with optimal control research has been carried out in the aerospace community [15], engineers from other disciplines and backgrounds still need to be involved into the subject. The idea of this work is to introduce these methods by addressing and formulating a few problems pertaining to different engineering fields in the realm of continuous dynamic optimization theory. The present article attempts to draw a concise introduction to the direct orthogonal collocation method. The transcription of the dynamic optimization problem (infinite-dimensional problem) into a finite-dimensional discrete NLP problem is mainly emphasized. Among others, LGR points are chosen for the collocation procedure. Hints on the numerical implementation are also given and the equivalence between the differential and integral forms is shown. The resulting NLP problems can be solved with dedicated open-source or commercial software [16], or by applying qualitatively different approaches such as evolutionary algorithms or meta-heuristics [17]. Moreover, a few historical engineering problems have been revisited, numerically solved and solutions have been compared with the ones available in the literature. Finally, conclusions are drawn and potential applications to two classes of dynamic optimization problems are summarized.

2. Mathematical Preliminaries

In this section the theoretical tools needed to develop the numerical framework are recalled. As a preliminary remark, note that all the optimization problems considered in this paper are defined in a finite interval. Without loss of generality, the numerical framework is developed with respect to $[-1, 1]$ to which any finite interval can be mapped by a linear transformation.

2.1 Legendre polynomials

Legendre polynomials are a system of polynomial functions with several applications in physics and engineering. More precisely, they are a countable set of polynomials, herein denoted by P_0, P_1, P_2, \dots which are the solutions to Legendre's differential equation [18]

$$\frac{d}{d\tau} \left[(1 - \tau^2) \frac{d}{d\tau} P_k(\tau) \right] + k(1 + k)P_k(\tau) = 0 \tag{1}$$

over the interval $\tau \in [-1, 1]$ (with $k = 0, 1, 2, 3, \dots$). Their explicit expression can be obtained by setting [18]

$$\begin{cases} P_0 = 0 \\ P_1 = \tau \end{cases} \tag{2}$$

and by the recurrence relation

$$(1 + k)P_{k+1}(\tau) = (1 + 2k)\tau P_k(\tau) - kP_{k-1}(\tau), \quad k = 2, 3, 4, \dots \tag{3}$$

An important property of Legendre polynomials they are orthogonal to one another, namely they have the following property

$$\int_{-1}^1 P_i(\tau)P_j(\tau) d\tau = \frac{2\delta_{ij}}{1 + 2j} \tag{4}$$

where δ_{ij} is Kronecker's delta.

2.2 Lagrange interpolating polynomials

Lagrange interpolating polynomials are used to approximate a function $f: \mathbb{R} \rightarrow \mathbb{R}$ whose values in a finite set of distinct points $\tau_1, \tau_2, \dots, \tau_j$ are known. They are defined by [18]

$$L_i(\tau) = \prod_{j=1, j \neq i}^J \frac{\tau - \tau_j}{\tau_i - \tau_j}, \quad i = 1, 2, \dots, J \tag{5}$$

and the approximation to which they lead can be written as

$$f(t) \approx \tilde{f}(t) = \sum_{j=1}^J f(\tau_j) L_j(t) \tag{6}$$

Note that since each L_j is a polynomial of degree J , so is \tilde{f} . As a consequence, $\tilde{f} \equiv f$ whenever f is a polynomial of degree less than or equal to J . Moreover, if f is a polynomial of degree less than or equal to J then

$$\frac{d}{dt} f(t) = \sum_{j=1}^J f(\tau_j) \frac{d}{dt} L_j(t)$$

From eq. (5) it is easy to see that each polynomial satisfies the so-called isolation property, i.e.,

$$L_i(\tau_j) = \delta_{ij} \tag{7}$$

As mentioned above, the pseudospectral methods described in the following sections are developed for the interval $[-1, 1]$. Hence the restriction of the polynomials to this interval will be of interest. Moreover, all the interpolation points will belong to this interval with, in particular, $\tau_1 = -1$ and $\tau_j = 1$.

2.3 Legendre-Gauss-Radau (LGR) points and quadrature weights

For a fixed $N \in \mathbb{N}$, the N Legendre-Gauss-Radau (LGR) collocation points are the roots of the polynomial $P_{N-1} + P_N$ [19], where P_{N-1} and P_N are the Legendre polynomial (of degree $N - 1$ and N , see eq. (2) and eq. (3)). An important property of the LGR points is that for any polynomial ϕ of degree $2(N - 1)$ or less [19], the identity

$$\int_{-1}^1 \phi(\tau) d\tau = \sum_{i=1}^N \omega_i \phi(\tau_i) \tag{8}$$



where ω_i ($i = 1, 2, \dots, N$) are the LGR quadrature weights, given by [19]

$$\omega_1 = \frac{2}{N^2}, \quad \omega_i = \frac{1}{(1 - \tau_i) \left[\frac{d}{d\tau} P_{N-1}(\tau_i) \right]^2}, \quad i = 2, 3, \dots, N \tag{9}$$

holds true.

2.4 Employed notation

Firstly, the noncollocated point $\tau_{N+1} = 1$ is introduced. All vector functions of τ are row vectors. For instance, the state and the control vectors at τ are written as $\mathbf{x}(\tau) = [x_1(\tau), x_2(\tau), \dots, x_n(\tau)] \in \mathbb{R}^n$ and $\mathbf{u}(\tau) = [u_1(\tau), u_2(\tau), \dots, u_m(\tau)] \in \mathbb{R}^m$, where n and m are the number of states and controls, respectively. The approximations of the state and the control at $\tau = \tau_i$ are denoted by \mathbf{X}_i and \mathbf{U}_i , respectively. Moreover, the matrix $\mathbf{X} \in \mathbb{R}^{(N+1) \times n}$ refers to the state approximation, where the first N rows contain the approximations at the collocated points $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_N$ and the last row contains the approximation at the noncollocated point \mathbf{X}_{N+1} . Analogously, the matrix $\mathbf{U} \in \mathbb{R}^{N \times m}$ refers to the control approximation, whose rows are \mathbf{U}_i ($i = 1, 2, \dots, N$). Finally, the notation $\mathbf{X}_{i:j}$ will be used to denote rows i through j of \mathbf{X} , while the $\mathbf{D}_{i:j}$ and $\mathbf{A}_{i:j}$ denote columns i through j of the differentiation and integration matrices, respectively, which are defined below.

3. Problem Formulation

The most general form of representing dynamic optimization problems is accomplished for by considering the so-called Bolza problem [20]:

Problem 1 (Original Problem)

$$\begin{aligned} \min_{\mathbf{u}(t) \in \tilde{\mathcal{C}}([t_0, t_f], \mathbb{R}^m)} \quad & J = \mathcal{M}(t_0, t_f, \mathbf{x}(t_0), \mathbf{x}(t_f)) + \int_{t_0}^{t_f} \mathcal{L}(t, \mathbf{x}(t), \mathbf{u}(t)) dt \\ \text{such that} \quad & \dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t)) \\ & \mathbf{x}(t_0) = \mathbf{x}_0 \\ & \mathbf{x}(t_f) = \mathbf{x}_f \\ & \mathbf{x}_L \leq \mathbf{x} \leq \mathbf{x}_U \\ & \mathbf{u}_L \leq \mathbf{u} \leq \mathbf{u}_U \\ & \mathbf{c}(t, \mathbf{x}(t), \mathbf{u}(t)) \leq \mathbf{0} \end{aligned} \tag{10}$$

where $\tilde{\mathcal{C}}([t_0, t_f], \mathbb{R}^m)$ denotes the set of piece-wise continuous functions from $[t_0, t_f]$ to \mathbb{R}^m . Besides, t denotes the time, but it can also be a spatial independent variable along which the state \mathbf{x} evolves according to a differential equation. In particular, t_0 and t_f denote the initial and final time. The term J is the goal functional to be minimized and it is made of two parts. The first part $\mathcal{M}: \mathbb{R} \times \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ takes the name of Mayer term and represents a punctual term at either t_0 or t_f , or both. The second part is called the Lagrange term and it is a distributed cost associated with the whole time domain $t \in [t_0, t_f]$ with the integrand function $\mathcal{L}: [t_0, t_f] \times \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}$. The minimization problem takes place within a specific dynamics $\dot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x}, \mathbf{u})$ with $\mathbf{f}: [t_0, t_f] \times \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^n$, given the initial \mathbf{x}_0 and final \mathbf{x}_f conditions. Finally, states and controls may be considered evolving between lower (subscript L) and upper (subscript U) bounds and obeying inequality path constraints, with $\mathbf{c}: [t_0, t_f] \times \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^p$.

Remark 1. As far as maximization problems are concerned, the aforementioned formulation is still valid provided that J is replaced by $-J$.

Remark 2. In a generic optimization problem, not all initial and final conditions may necessarily be given. Moreover, either t_0 or t_f (or both) may be free. If some of these quantities are fixed, then they cannot be decision variables and hence they must be dropped from the set of arguments of \mathcal{M} .

Problem 1 represents a generic constrained continuous dynamic optimization problem in the physical domain $t \in [t_0, t_f]$. The aim of the transcription procedure is that mapping it into a non-linear (constrained) programming problem that can be solved by using NLP tools. To ease the exposition of the transcription into a NLP problem, the following reduced unconstrained dynamic optimization problem in the pseudospectral domain $\tau \in [-1, 1]$ is considered:

Problem 2 (Reduced Problem)

$$\begin{aligned} \min_{\mathbf{u}(\tau) \in \tilde{\mathcal{C}}([-1, 1], \mathbb{R}^m)} \quad & J = \mathcal{M}(\mathbf{x}(1)) + \frac{t_f - t_0}{2} \int_{-1}^1 \mathcal{L}(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau \\ \text{such that} \quad & \dot{\mathbf{x}}(\tau) = \mathbf{f}(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau)) \\ & \mathbf{x}(-1) = \mathbf{x}_0 \end{aligned} \tag{11}$$

Here, \mathbf{x}_0 , t_0 and t_f are assumed to be given. Below, it is emphasized that the transcription process for Problem 1 is not much different from that of Problem 2. Moreover, solutions for Problem 2 can be transformed into solutions for Problem 1 by taking into account the affine transformations from and to the original and the pseudospectral intervals, namely

$$\begin{cases} t = \frac{t_f - t_0}{2} \tau + \frac{t_f + t_0}{2} \\ \tau = \frac{2}{t_f - t_0} t - \frac{t_f + t_0}{t_f - t_0} \end{cases} \tag{12}$$

In the following, the reduced problem (Problem 2) is transcribed into a constrained NLP problem using Legendre-Gauss-Radau pseudospectral method.



4. Legendre-Gauss-Radau Pseudospectral Method

According to [4], the minimum fundamental steps of a transcription consist of the domain discretization, the continuous-to-discrete conversion of states and/or controls and the characterization of differential and integral forms of the considered pseudospectral method, possibly making sure these latter are equivalent. Hereinafter, following [21], a systematic mathematical framework is devoted to each of the above mentioned three steps. The reader is also addressed to other variants of this formulation where flipped LGR points $P_N(\tau) - P_{N-1}(\tau)$, namely the negative of the standard LGR points) are considered (see, e.g., [4, 22, 23]).

4.1 Continuous-to-discrete conversion: Discretization and collocation

Consider collocation at the N LGR points $(\tau_1, \tau_2, \dots, \tau_N)$ with $\tau_1 = -1$ and let $\tau_{N+1} = 1$ be the non-collocated point. The evolution of each state is approximated by a polynomial of degree N through Lagrange interpolation polynomials, i.e.,

$$\mathbf{x}(\tau) \approx \mathbf{X}(\tau) = \sum_{i=1}^{N+1} \mathbf{X}_i L_i(\tau) \tag{13}$$

where, according to eq. (5),

$$L_i(\tau) = \prod_{j=1, j \neq i}^{N+1} \frac{\tau - \tau_j}{\tau_i - \tau_j}, \quad i = 1, 2, \dots, N + 1 \tag{14}$$

It is worth noting that the state approximation in eq. (13) includes the Lagrange polynomial $L_{N+1}(\tau)$ (of degree N) associated with the non-collocated point τ_{N+1} . Differentiating eq. (13) and denoting by a dot the first derivative with respect to τ , one obtains

$$\dot{\mathbf{x}}(\tau) \approx \dot{\mathbf{X}}(\tau) = \sum_{i=1}^{N+1} \mathbf{X}_i \dot{L}_i(\tau) \tag{15}$$

which is a polynomial of degree $N + 1$. Evaluating eq. (15) at the generic collocation point τ_j ($j = 1, 2, \dots, N$), one obtains

$$\dot{\mathbf{X}}(\tau_j) = \sum_{i=1}^{N+1} D_{ji} \mathbf{X}_i \tag{16}$$

where $D_{ji} = \dot{L}_i(\tau_j)$. Moreover, taking into account the right-hand side of the dynamics in Problem 2 at the collocation points, the approximations \mathbf{X}_i are found imposing

$$\sum_{i=1}^{N+1} D_{ji} \mathbf{X}_i = \frac{t_f - t_0}{2} \mathbf{f}(\tau_j, \mathbf{X}_j, \mathbf{U}_j), \quad j = 1, 2, \dots, N \tag{17}$$

According to the notation specified in Section 2.4, letting

$$\mathbf{X}_{1:N} = \begin{bmatrix} \mathbf{X}_1 \\ \vdots \\ \mathbf{X}_N \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} \mathbf{X}_{1:N} \\ \mathbf{X}_{N+1} \end{bmatrix}, \quad \mathbf{F}_{1:N} = \begin{bmatrix} \mathbf{f}_1 \\ \vdots \\ \mathbf{f}_N \end{bmatrix}$$

where $\mathbf{f}_i = \frac{t_f - t_0}{2} \mathbf{f}(\tau_i, \mathbf{X}_i, \mathbf{U}_i)$, Equation (17) may be written in a more compact form as

$$\mathbf{D}\mathbf{X} = \mathbf{F}_{1:N} \tag{18}$$

where $\mathbf{D} \in \mathbb{R}^{N \times (N+1)}$ is the non-square differentiation matrix whose entries are the coefficients D_{ji} . The extra column of \mathbf{D} is due to the Lagrange polynomial at the noncollocated point $\tau_{N+1} = 1$. Letting \mathbf{D}_1 and $\mathbf{D}_{2:N+1}$ denote the vector containing the first column and the matrix containing the remaining N columns of the differentiation matrix \mathbf{D} , respectively, the compact form of collocation eq. (18) may be written as

$$\mathbf{D}_1 \mathbf{X}_1 + \mathbf{D}_{2:N+1} \mathbf{X}_{2:N+1} = \mathbf{F}_{1:N} \tag{19}$$

Hence, recalling eq. (8), Problem 2 may be transcribed into the following discrete NLP problem:

Problem 3 (Equivalent NLP Problem)

$$\begin{aligned} \min_{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{N+1}, \mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_N} \quad & J = \mathcal{M}(\mathbf{X}_{N+1}) + \frac{t_f - t_0}{2} \sum_{i=1}^N \omega_i \mathcal{L}_i \\ \text{such that} \quad & \mathbf{D}_1 \mathbf{X}_1 + \mathbf{D}_{2:N+1} \mathbf{X}_{2:N+1} = \mathbf{F}_{1:N} \\ & \mathbf{X}_1 - \mathbf{x}_0 = \mathbf{0} \end{aligned} \tag{20}$$

where $\mathcal{L}_i = \mathcal{L}(\tau_i, \mathbf{X}_i, \mathbf{U}_i)$. Problem 3 is a finite-dimensional NLP constrained problem, whose decision variables are the approximation of the state at the LGR points plus the final point and the control only at the LGR points. Moreover, it is appreciated that the summation term in Problem 3 gives an exact value of the integral term in Problem 2 whenever \mathcal{L} is of degree at most $2(N - 1)$ [19].

Remark 3. It is important to observe that collocation equations (equality constraints) include the N LGR points plus the final point $\tau_{N+1} = 1$. This aspect yields a neat setup of the problem with respect to that obtained by the LG pseudospectral method [6, 24], where an additional equation is inevitably required for the evaluation of the state, and hence the Mayer term \mathcal{M} , at $\tau = 1$.

Remark 4. The aforementioned conversion can be done for problems including upper, lower and path constrains. In particular, if the quantities



$$\mathbf{C}_{1:p} = \begin{bmatrix} c_1(\tau_i, \mathbf{X}_i, \mathbf{U}_i) \\ \vdots \\ c_p(\tau_i, \mathbf{X}_i, \mathbf{U}_i) \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} \mathbf{C}_{1:p} \\ \mathbf{X} - \mathbf{x}_U \\ -\mathbf{X} + \mathbf{x}_L \\ \mathbf{U} + \mathbf{u}_U \\ -\mathbf{U} + \mathbf{u}_L \end{bmatrix}$$

are introduced at the collocation points ($i = 1, 2, \dots, N$), the vector \mathbf{C} can be added to the NLP as an inequality constraint.

4.2 Hints on numerical implementation

The correspondence between Problem 3 and standard NLP problems is briefly addressed. A different notation from that introduced in Section 2.4 and compatible with the conventional formulation of an NLP problem is required. To this purpose, let $\mathbf{Y}_j \in \mathbb{R}^{N+1}$ ($j = 1, 2, \dots, n$) and $\mathbf{V}_i \in \mathbb{R}^N$ ($i = 1, 2, \dots, m$) denote the generic columns of the state and control approximation matrices \mathbf{X} and \mathbf{U} , respectively. Let also

$$\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_1 \\ \mathbf{Y}_2 \\ \vdots \\ \mathbf{Y}_n \end{bmatrix} \in \mathbb{R}^{n(N+1)}, \quad \mathbf{V} = \begin{bmatrix} \mathbf{V}_1 \\ \mathbf{V}_2 \\ \vdots \\ \mathbf{V}_m \end{bmatrix} \in \mathbb{R}^{mN}$$

be the generalized state and control approximation vectors. The decision variables of Problem 3 may therefore be collected in the following vector

$$\mathbf{Z} = \begin{bmatrix} \mathbf{Y} \\ \mathbf{V} \\ t_0 \\ t_f \end{bmatrix} \in \mathbb{R}^{n(N+1)+mN+2}$$

-serving as the vector of decision variables for the NLP problem. Hence, the reshape of the goal function and equality constraints in Problem 3 (and possibly upper, lower and path constraints in Problem 1) in terms of \mathbf{Z} is straightforward by the aid of Remark 4. For further details, the reader is addressed to the well-known studies, e.g., [25-30].

4.3 Integral formulation

The pseudospectral discretization of the state described above admits an equivalent integral formulation which avoids the loss of information due to the discretization of the input term and which is described next. To begin with, note that, for any j such that $1 < j \leq N + 1$, one may write

$$\mathbf{x}(\tau_j) = \mathbf{x}(-1) + \frac{t_f - t_0}{2} \int_{-1}^{\tau_j} \mathbf{f}(\mathbf{x}(\zeta), \mathbf{u}(\zeta)) d\zeta \tag{21}$$

By replacing the integral variable ζ by the variable $\sigma = \frac{2(\zeta+1)}{\tau_j+1} - 1$, eq. (21) may be written as

$$\mathbf{x}(\tau_j) = \mathbf{x}(-1) + \left(\frac{t_f - t_0}{2}\right) \left(\frac{\tau_j + 1}{2}\right) \int_{-1}^1 \mathbf{f}(\mathbf{x}(\sigma), \mathbf{u}(\sigma)) d\sigma \tag{22}$$

leading to the approximation

$$\mathbf{x}(\tau_j) \approx \mathbf{x}(-1) + \sum_{i=1}^N \frac{t_f - t_0}{2} \alpha_{ji} \mathbf{f}_i \tag{23}$$

where weights α_{ji} are equal to $\frac{\tau_j+1}{2} \omega_i$ (with $j = 2, 3, \dots, N + 1$). In conclusion, denoting by $\mathbf{1}$ a column vector of ones and by \mathbf{A} the integration matrix of entries $\alpha_{i,j}$ and letting $\mathbf{A}_{2:N+1}$ be the second through the $(N+1)$ -th column submatrix of \mathbf{A} , the state approximation (23) at $\tau_j > \tau_1$ can be recast in the compact form

$$\mathbf{X}_{2:N+1} = \mathbf{1}\mathbf{X}_1 + \mathbf{A}_{2:N+1}\mathbf{F}_{1:N} \tag{24}$$

Note that, provided that $\mathbf{D}_{2:N+1}$ is non-singular, eq. (19) can be rearranged as

$$\mathbf{X}_{2:N+1} = -\mathbf{D}_{2:N+1}^{-1}\mathbf{D}_1\mathbf{X}_1 + \mathbf{D}_{2:N+1}^{-1}\mathbf{F}_{1:N} \tag{25}$$

which, compared with the integral form of collocation equations (24), leads to the conclusion that the two formulations are equivalent if

$$\mathbf{D}_{2:N+1}^{-1} = \mathbf{A}_{2:N+1} \tag{26}$$

and

$$\mathbf{1} = \mathbf{D}_{2:N+1}^{-1}\mathbf{D}_1 \tag{27}$$

Requirements (26) and (27) can be proved within the following reasoning (see [8, 9]). Firstly, from the construction of \mathbf{D} , the components of \mathbf{D}_1 are all zero since they are the derivatives at the collocation points of the polynomial whose value is 1 at τ_i , $1 \leq i \leq N + 1$. As a consequence, the first column of \mathbf{D} is given by

$$\mathbf{D}_1 = -\sum_{j=2}^{N+1} \mathbf{D}_j = \mathbf{D}_{2:N+1}\mathbf{1} \tag{28}$$

Note that the second requirement (27) is satisfied by pre-multiplying eq. (28) by $\mathbf{D}_{2:N+1}^{-1}$, provided that this latter is nonsingular. To show this latter, let $\mathbf{v} \in \mathbb{R}^{N+1}$ be a nonzero column vector whose first component, v_1 , is equal to zero and for which $\mathbf{D}\mathbf{v} = \mathbf{0}$. Moreover, let $\phi(\tau)$ be the unique polynomial of degree N which satisfies $\phi(\tau_i) = v_i$, $1 \leq i \leq N + 1$. Since the components of $\mathbf{D}\mathbf{v}$ are the derivative of ϕ evaluated at the collocation points and since ϕ is a polynomial of degree $N - 1$, it must be identically zero since it vanishes at N points. Hence, ϕ is a constant. Since $\phi(-1) = 0$, therefore ϕ is identically zero as well, implying that $\mathbf{D}\mathbf{v} = \mathbf{0}$ with $v_1 = 0$ has no nonzero solution, from which the nonsingularity of $\mathbf{D}_{2:N+1}$ is established.



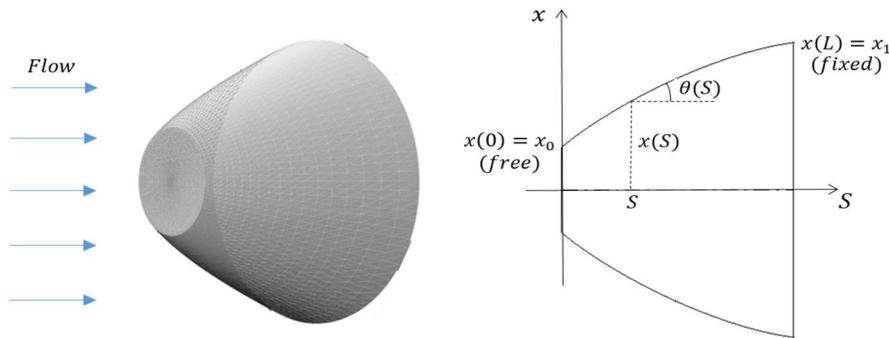


Fig. 1. A schematic representation of a body of revolution moving through a fluid and definition of employed variables.

Moreover, pre-multiplying eq. (24) by $D_{2:N+1}$ and recalling eq. (27), it yields

$$D_1 X_1 + D_{2:N+1} X_{2:N+1} = D_{2:N+1} A_{2:N+1} F_{1:N} \tag{29}$$

Finally, recalling eq. (18), it follows

$$D_{2:N+1} X_{2:N+1} = I \tag{30}$$

where I is the $N \times N$ identity matrix, from which the first requirement (26) is derived.

Remark 5. It is worth noting that, unlike pseudospectral methods using LG and LGR points, the LGL method suffers from the absence of the above mentioned equivalence of both differential and integral forms. This is because the derivative is collocated at all the LGL discretization points ($\tau_1 = -1, \tau_2, \dots, \tau_N = 1$), leading to a singular square differentiation matrix (for mathematical justifications, see [31]).

5. Application and Discussion

In this section, a few continuous dynamic optimization problems pertaining to different disciplines in engineering are illustrated, numerically solved and discussed. Optimal solutions are obtained by the method presented above and are compared to either analytical or numerical solutions derived by other two numerical methods. In the first one (the shooting method, which pertains to indirect methods), both states and constants at the endpoint t_f are guessed and a forward integration of the necessary conditions for optimal solutions as an initial value problem is performed. A check is then made whether the corresponding boundary values are satisfied. If so, a solution is found, if not the initial guesses are adjusted. In the second one (the steepest descent method), the philosophy is basically to reformulate and solve the original problem as a boundary value problem. In particular, a sequence of problems in which one or more of the necessary conditions for optimal solutions is initially violated, but eventually satisfied if the iterative procedure converges. Here, the step size is set as a constant and selected with a line search method which maximizes the reduction of performance measure in each iteration. It is worth noting that the iterative procedure in all methods terminates when $|J^{i+1} - J^i| \leq 10^{-6}$. Finally, solutions associated with the present method are derived by imposing $N = 20$.

5.1 Newton's body

Newton's famous problem of finding the optimal shape of a solid body of revolution which moves through a resisting medium in the direction of its axis of revolution with the least possible resistance is addressed [32]. Notwithstanding Newton's model for the fluid was wrong as per our current understanding, it finds well agreements with experimental data at hypersonic speeds [33].

Consider an axisymmetric body moving through a homogeneous fluid (see Fig. 1). Let $S \in [0, L]$ be the coordinate taken on the axial direction, $x(S) \in [x_0, x_1]$ be the meridian profile normalized with respect to the axial length L . Let also $\theta(S)$ the angle between the tangent at point $(S, x(S))$ and the S -axis. Introducing the normalized variable $t = S/L \in [0, 1]$, and letting $u(t) = \frac{dy(t)}{dt} = \tan \theta(t)$, the formulation of the optimization problem is the following [34]:

$$\begin{aligned} \min_{u \in \tilde{C}([0,1], \mathbb{R})} \quad & \tilde{D} = x_0^2 + 2 \int_0^1 \frac{x(t)u(t)^3}{1 + u(t)^2} dt \\ \text{such that} \quad & \dot{x}(t) = u(t) \\ & x(1) = x_1 \end{aligned} \tag{31}$$

where \tilde{D} is the the normalized drag force, which is the performance index to be minimized, while x_0 and x_1 are the maximal and minimal normalized radii, at $t = 0$ and $t = 1$, respectively. If $x_0 \neq 0$, the body is said to have a blunt tip. Explicit solutions can be obtained by means of calculus of variations when x_0 is fixed and the so-called arc-of-length (AoL) assumption ($u \ll 1$ or $1 + u^2 \ll 1$) holds, namely [35]

$$x(t) = [x_0^{4/3} + (x_1^{4/3} - x_0^{4/3})t]^{3/4} \tag{32}$$

otherwise, solutions can be derived in a parametric form in terms of $1/u$, i.e., $t = t(1/u)$ and $x = x(1/u)$, as follows [34]:

$$t(1/u) = \frac{x_0}{4} \left(\frac{3}{4u^4} + \frac{1}{u^2} - \ln(1/u) - \frac{7}{4} \right), \quad x(1/u) = \frac{x_0}{4} \frac{(1 + 1/u^2)^2}{1/u} \tag{33}$$



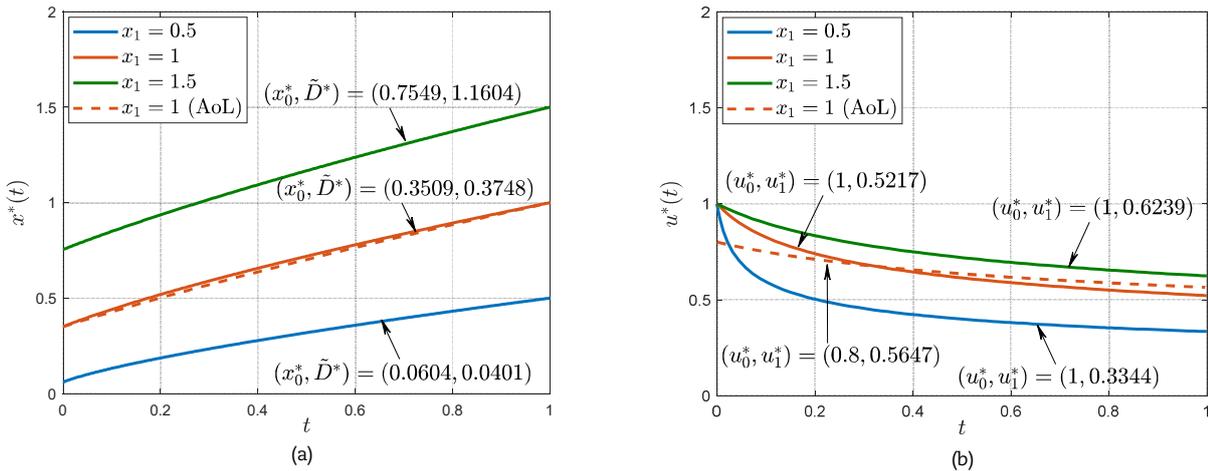


Fig. 2. (a) Optimal meridian profiles for Newton's body with different values of x_1 by means of the LGR method (solid lines) and the analytical closed-form solution in eq. (32) with $x_1 = 1$ (dashed line). (b) Optimal input functions with illustration of the Weierstrass-Erdmann condition at $t = 0$.

Besides, it is worth noting that the Weierstrass-Erdmann condition at the blunt tip should be satisfied, i.e., [34]

$$u_0 = 1 \tag{34}$$

Moreover, denoting by u_1 the slope of the meridian profile at $t = 1$, it can be shown that u_1 and x_0 are the solution of the following system of transcendental equations [34]

$$\frac{3}{4u_1^4} + \frac{1}{u_1^2} - \ln(1/u_1) - \frac{7}{4} = \frac{(1 + 1/u_1^2)^2}{1/u_1}, \quad x_0 = \frac{4x_1/u_1}{(1 + 1/u_1^2)^2} \tag{35}$$

Finally, the optimal normalized drag force is analytically given by

$$\bar{D} = \frac{u_1^2 x_1^2 \{2u_1^6 + [17 - 4 \ln(u_1)]u_1^4 + 10u_1^2 + 3\}}{2(1 + u_1^2)^4} \tag{36}$$

For the sake of giving an example, if $x_1 = 1$, the system of equations (35) yields $u_1 = 0.5216$ and $x_0 = 0.3509$. Numerical results obtained by the application of the present method have shown good agreement with the above values. Figure 2 shows optimal states (meridian profile) and control functions (their derivative with respect to t) associated with different values of x_1 . Moreover, the optimal profile corresponding to the AoL assumption obtained by using eq. (32) and employing the above mentioned value of x_0 is also depicted for comparison. Optimal performance indices are listed for each solution and are in agreement with eq. (36) to four digits after the decimal point and therefore with analytical solutions. Also, it is worth highlighting that numerical results satisfy the condition (34).

5.2 Lagrange's column

The problem of determining the shape of a simply supported column loaded by concentrated forces at its ends having maximum buckling load F for given volume was formulated by Lagrange in 1773 [34]. Mathematically, this amounts to the maximization of the eigenvalue of a certain Sturm-Liouville problem subject to an isoperimetric constraint. Clausen in 1851 solved the problem for columns of circular cross section pinned at the end points, yet in this solution optimal cross sectional area vanishes at end points [36]. The solution of the problem was also obtained by many other authors, e.g., [37-39]. In Ref. [40], it has been highlighted that the optimal solution for Lagrange's problem and its dual version (minimization of the volume for a given buckling load) are the same, provided that the static equations are linearized.

Due to symmetry, the problem can be solved considering half, but cantilevered, column. Therefore, the optimization problem reads [40]:

$$\begin{aligned} & \min_{u \in C([0,1], \mathbb{R})} && F = -x_4(1/2) \\ & \text{such that} && \dot{x}_1(t) = x_2(t)/u(t)^2 \\ & && \dot{x}_2(t) = -x_1(t)x_4(t) \\ & && \dot{x}_3(t) = u(t) \\ & && \dot{x}_4(t) = 0 \\ & && x_1(1/2) = x_2(0) = x_3(0) = 0 \\ & && x_3(1/2) = a \\ & && u(t) \geq \bar{u} \end{aligned} \tag{37}$$

where, x_1 and x_3 denote the cross-section rotation angle and the normalized rate of change of the volume, respectively, while x_2 and x_4 are auxiliary state variables proportional to the bending moment and the buckling load, respectively. Here, the control function u refers to the cross-sectional area distribution along the axis and a is the half volume of the column.

In Ref. [40], the problem has been numerically solved by using the shooting method and considering $a = 0.433$ to obtain $F^* = -x_4^*(1/2) = -9.869 \approx -\pi$, so it is compared to slender columns of unit length and unit volume with uniform distribution of material along the column axis (i.e., the minus sign apart, it is the critical load according to Euler's formula). Optimal solutions, however, suffer from Clausen-type behavior, namely vanishing at the free end. By employing the direct transcription method, the problem can be solved for arbitrary values of $\bar{u} > 0$, which denotes the minimal cross-sectional area. For $\bar{u} = 0$ (Clausen's solution) it was shown that states behave more or less similarly along the column axis (see Fig. 3), whereas the difference between the optimal cross sectional area distribution and that obtained by the shooting method is marginal (see Fig. 4).



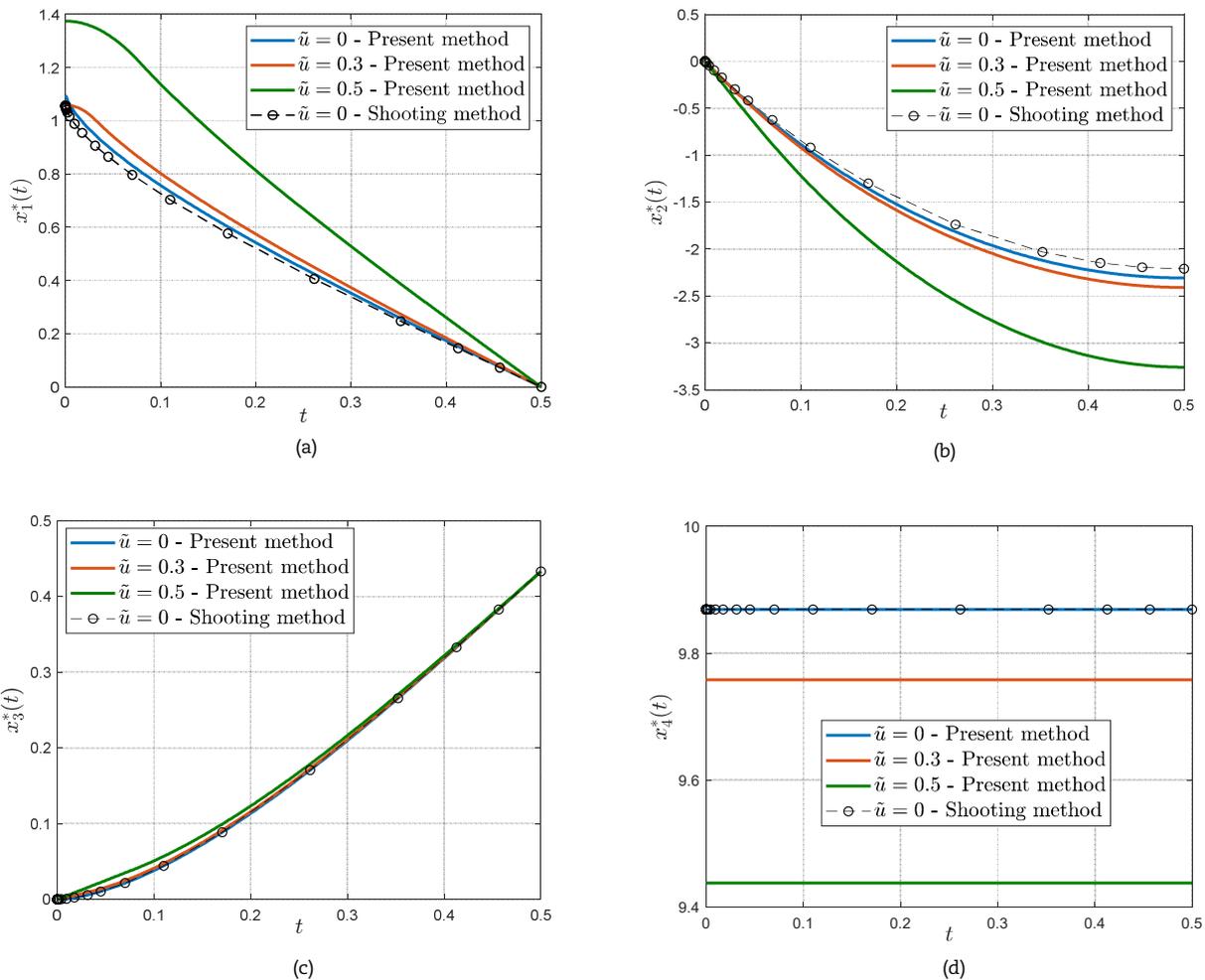


Fig. 3. Optimal states for Lagrange's column with different constraints on the minimal value of the control function \tilde{u} .

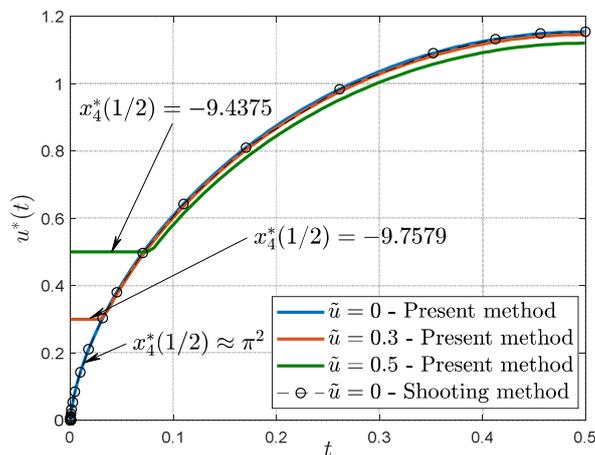


Fig. 4. Optimal cross-sectional area distributions for Lagrange's column with different constraints on the minimal value of the control function \tilde{u} .

The assumption that $u(t) \geq \tilde{u}$ has been easily included in the present method by considering an inequality constraint on the control function at each LGR point. Corresponding optimal solutions consist of an interval where the optimal control function is constant and then monotonically increasing, reaching the maximum value at $t = 1/2$, i.e., at the fixed end of the cantilever (or at the central point of the simply supported column). Moreover, since a is fixed ($a = 0.433$), $u^*(1/2)$ decreases as \tilde{u} increases.

5.3 Continuous stirred-tank chemical reactor

The control of a continuous stirred-tank chemical reactor as originally formulated in [41] and revisited in [42] is now considered. A first-order, irreversible exothermic reaction is carried out in the reactor and the control is to be achieved by the manipulation of the flow of cooling fluid through a cooling coil inserted in the reactor. The states of the plant are x_1 and x_2 , denoting the temperature and concentration deviations from their steady-state values, respectively, while the control u is the effect of the coolant flow on the chemical reaction. Here, the independent variable t denotes the time.



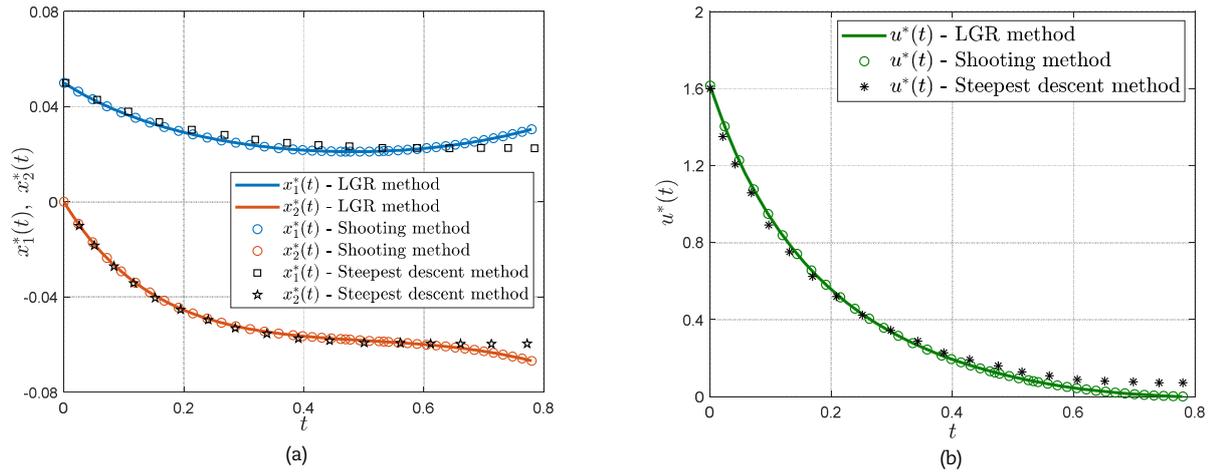


Fig. 5. (a) Optimal states and (b) the optimal control for the continuous stirred-tank chemical reactor with LGR (solid lines) and with the shooting and steepest descent (scattered points) methods.

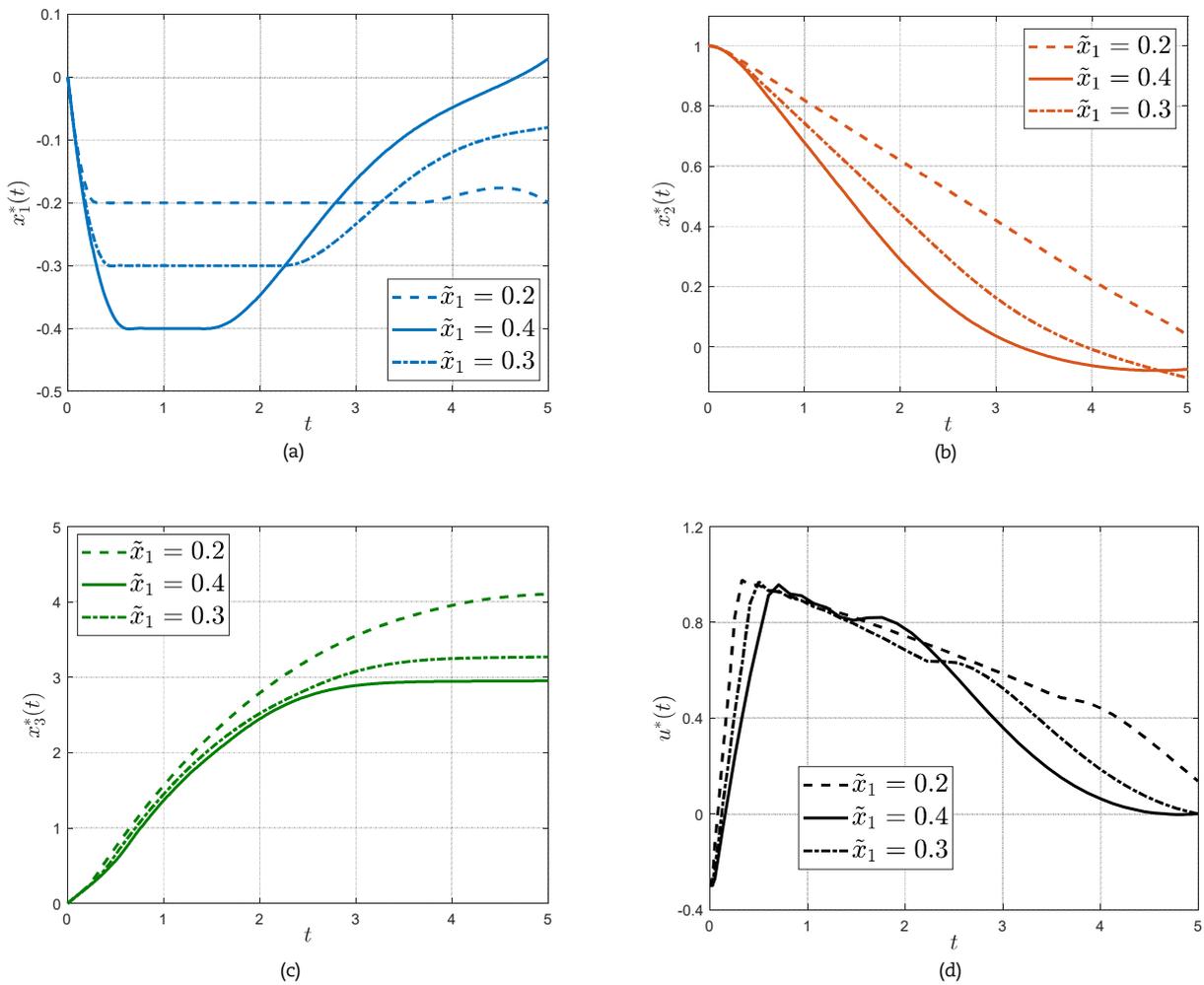


Fig. 6. (a, b, c) Optimal states and (d) input function for the Van der Pol oscillator problem with three constraints on the minimal value of the state x_1 .

If one is interested that the desired objective is to maintain the temperature and concentration close to their steady state values without expending large amount of control effort, then the optimization problem may be stated as follows [43]:

$$\begin{aligned}
 & \min_{u \in \mathcal{C}([0,0.78], \mathbb{R})} E = \int_0^{0.78} [x_1(t)^2 + x_2(t)^2 + Ru(t)^2] dt \\
 & \text{such that} \quad \dot{x}_1(t) = -[2 + u(t)][x_1(t) + 0.25] + [x_2(t) + 0.5] \exp\left(\frac{25x_1(t)}{x_1(t) + 2}\right)
 \end{aligned} \tag{38}$$



$$\begin{aligned}\dot{x}_2(t) &= 0.5 - x_2(t) - [x_2(t) + 0.5] \exp\left(\frac{25x_1(t)}{x_1(t) + 2}\right) \\ x_1(0) &= 0.05 \\ x_2(0) &= 0\end{aligned}$$

where E is an overall energy measure and R is an arbitrary weighing factor, which is chosen to be 0.1. As it is shown in Fig. 5, numerical solutions for the states and input function obtained by the shooting method and the LGR method show a good agreement, whereas solutions associated with the steepest descent method presents a discernible difference. Optimal values of E , i.e., E^* , are equal to 0.0290, 0.0282 and 0.0266 when the shooting, steepest descent and LGR pseudospectral methods are employed, respectively, indicating that the performance index is rather insensitive to states and control variations in the vicinity of the optimum solution.

5.4 Van der Pol oscillator

Van der Pol circuits are electric self-oscillating triode circuits originally used for signal transmission and receipt, whose oscillatory behavior is governed by a second-order nonlinear differential equation. A fixed final time formulation of the Van der Pol oscillator with path constraints on states and inputs is given by [44, 45]:

$$\begin{aligned}\min_{u \in C([0,5], \mathbb{R})} \quad & J = x_3(5) \\ \text{such that} \quad & \dot{x}_1(t) = (1 - x_2(t)^2)x_1(t) - x_2(t) + u(t) \\ & \dot{x}_2(t) = x_1(t) \\ & \dot{x}_3(t) = x_1(t)^2 + x_2(t)^2 + u(t)^2 \\ & x_1(0) = 0 \\ & x_2(0) = 1 \\ & x_3(0) = 0 \\ & x_1(t) \geq -\tilde{x}_1 \\ & -0.3 \leq u(t) \leq 1\end{aligned} \tag{39}$$

Also here, the independent variable t denotes the time, while the state x_3 has been introduced to transform the cost functional from a distributed one (Lagrange cost) to a Mayer cost functional. Figure 6 shows numerical solutions for optimal states and input function for three instances of \tilde{x}_1 by means of the LGR method, complying with the path constraint on the state and the input function. Optimal values of J , i.e., $x_3^*(5)$, are equal to 4.1056, 3.2710 and 2.9538 for $\tilde{x}_1 = 0.2, 0.3$ and 0.4 , respectively.

6. Conclusion

Analytical solution to dynamic optimization problems from the first-order necessary conditions derived from principles of calculus of variations is a difficult task for most of the engineering applications. Numerical approximation to the solution, therefore, is mandatory. A numerical method is addressed in this article, which transcribes infinite-dimensional problems into finite-dimensional nonlinear programming problems based on the collocation of the dynamics equations at Legendre-Gauss-Radau discretization points. States are described in terms of Lagrange interpolating polynomials, while the distributed term in the performance index is approximated by quadrature. A few benchmark historical problems from different engineering backgrounds are recalled, numerically solved and thoroughly discussed. The present method yield numerical solutions that are in good agreement with those in literature and ambitiously expected to be adopted for dynamic optimization problems in engineering. A possible extension of the method could deal with uncertain models, for which recent results [46, 47] are promising.

Eventually, two possible classes of dynamic optimization problems in structural mechanics for which direct transcription methods can be potentially used are herein summarized. The first one concerns shape optimization problems arising in the realm of elastic rod theory. This class of problems has been being investigated by many researchers. Particular examples may range from the longest-reach bar [48-50] to the torsional shaft [51], Pflüger's rod [52], the rod lying on elastic foundations [53] and others, possibly modelled within the non-local elasticity [54]. Governing equations for these scenarios are the static equations and sound objective functions are the minimization of the rod volume, the maximization of the buckling load or the maximization of the free-end displacement. To the extent of the authors' knowledge, the overwhelming related studies exploit indirect methods referring to necessary conditions for optimal solutions for each problem separately, whereas the mathematical framework of direct transcription methods formally gives a chance to investigate them within a unified formalism. Another class of problems arises within the design of the so-called functionally graded materials, namely those non-homogeneous materials whose constituents' volume fractions gradually vary along a specific direction. This variation, in turn, is reflected into a variation of the mechanical, physical and thermal properties. In this case, the dynamics is given by the equations of linear elasticity. A recent analytical attempt has been carried out in [55, 56] for axisymmetric bodies to search for the best volume fractions such that maximum equivalent stresses attain their minimum values, under the application of internal pressure and subject to technological constraints, showing that optimal volume fractions are piecewise linear with respect to the radial coordinate. It will be interesting to numerically solve the problem beyond the analytical tractability and possibly including thermal loading.

Author Contributions

All authors made a substantial, direct and intellectual contribution to this work. The manuscript was written through the contribution of all authors. All authors discussed the results, reviewed, and approved the final version of the manuscript.

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Conflict of Interest

The authors declared no potential conflicts of interest with respect to the research, authorship, and publication of this article.



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Data Availability Statements

The datasets generated and/or analyzed during the current study are available from the corresponding author on reasonable request.

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