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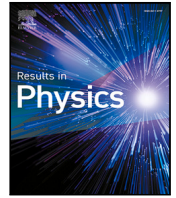
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Non-holonomic constraints: Considerations on the least action principle also from a thermodynamic viewpoint

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ABSTRACT

For the system with non-holonomic constraints, the principle of least action does not seem to lead to the equations describing the motion, which are consistent with the physical behaviour. Here, some considerations are developed on this fundamental topic in Mathematical Physics. Moreover, a thermodynamic approach is introduced based on the first and second laws of thermodynamics.

Introduction

The Principle of Least Action represents one of the most studied bases of Physics, and some controversies emerged during its historical development.

In two papers, dated 1741 and 1744, submitted to the French Academy of Sciences, Pierre-Louis Moreau de Maupertuis (1698–1759) [1] mentioned a *Principe de la moindre quantité d'action* (principle of least action), that he defined universally. In particular, he highlighted that when a change occurs in Nature, the Action required for that change is as small as possible. Then, Leonhard Euler (1707–1783) improved this result by pointing out that the real trajectory of any moving mass particle is the one, from among all possible trajectories connecting the same endpoint, that minimises the action, which he realised to be the time integral of the twice kinetic energy [2].

In the development of Mechanics, the method of least squares, introduced by Carl Friedrich Gauss (1777–1855), appeared first in the analysis of the elliptical orbit of the asteroid Ceres [3], strictly related to Legendre's approach. The improvement of this approach led to the formulation that, from all possible motions, the actual one leads under given conditions to the least constraint, a principle strictly related to d'Alembert's Principle (Jean d'Alembert, 1717–1783). In this context, a statistical mechanical analysis of Gauss' Principle has been developed concerning its application for holonomic (constraints depend only on co-ordinates) and non-holonomic (non-integrable constraints on velocity) constraints, pointing out that Gauss' principle is limited to arbitrary holonomic constraints and apparently, to non-holonomic constraint functions which are homogeneous functions of the momenta [4].

Nowadays, the principle of least action is used in Physics, even if it is often known as Hamilton's principle more than Maupertuis's

principle, while it does not find interest in engineering, where some variational principles are used for applications [5], even if an interest for the use of least action principle is growing in biomechanics and robotics [6]. The variational methods are fundamental in the development of modern analytical mechanics [7]. But, Flannery [7–10] pointed out:

“The least action principle can be applied only to holonomic and linear non-holonomic constraints, while it is not useful to obtain the correct equations of motion for general non-holonomic constraints”.

The problem pointed out by this statement can be summarised as the following question: Is it possible to prove that the principle of least action cannot be applied to general non-holonomic constraints?

In this paper, the problem of the validity of the least action principle is discussed to propose proof for answering the question pointed out by Flannery. To do so, in Materials and Methods section the holonomic and non-holonomic constraints are discussed, in the Results section a proof in relation to the Flannery question is proposed, and in the last section some considerations are developed from a Thermodynamic viewpoint.

Materials and methods

Preliminary considerations

The mechanical systems' movements are restricted by constraints due to material achievements which can be geometrically represented

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by lines, curves, planes, and surfaces [11]. The constraints are described by their mathematical equations and by the forces related to the binding reaction (physical description) [11].

In order to determine the spatial position of a system of N material points, the values of N position vectors \mathbf{r} are required, i.e. [12]:

- $3N$ coordinates $r_i, i \in [1, 3]$, if the system is free, i.e., the points representing the system are all possible;
- $n \leq 3N$ coordinates, if some of the points representing the system are subjected to restriction, and n is the number of the system's freedom degrees.

Consequently, for a general approach, it is convenient to introduce a system of $n \leq 3N$ (with $n = 3N$, if the system is free) generalised coordinates q appropriate to the problem considered [12]. The values of the generalised velocities are also required to determine the mechanical condition of a system at a given time: $(\mathbf{q}, \dot{\mathbf{q}})$, where $\mathbf{q} = (q_1, \dots, q_n)$ and $\dot{\mathbf{q}} = (\dot{q}_1, \dots, \dot{q}_n)$, at the same time [12].

In this context, the definition of constraint must be introduced as follows:

Definition 1 ([11]). A constraint is said:

1. Holonomic, if any restriction on the possible configurations of the system follows the condition:

$$f(\mathbf{q}, t) = 0 \quad (1)$$

which is an integrable relation;

2. Non-holonomic, if any restriction on the movements possible [11] of the system follows the condition:

$$g(\mathbf{q}; \dot{\mathbf{q}}, t) = 0 \quad (2)$$

which is not an integrable relation.

If the non-holonomic constraints represent a holonomic constraint, it is integrable.

Holonomic and Lagrangian systems

The concept of a map is fundamental to represent the domain of a real open set. Thus its definition must be introduced.

Definition 2 ([11]). Let Q be a set of points. It is said a map of size n on Q an application injective $\varphi : U \subseteq Q \rightarrow \mathbb{R}^n$, with the image the open set $\varphi(U)$ in \mathbb{R}^n . The n functions $Q_i : U \rightarrow \mathbb{R}, i \in [1, n]$, such that $\forall x \in U : \varphi(x) = (Q_1(x), \dots, Q_n(x))$, are the coordinates associated with the fold φ . The $\mathbf{q} = \{Q_i\}_{i \in [1, n]}$ form a local coordinate system on all Q . It denotes the fold with the pair (U, φ) or (U, \mathbf{q}) .

In this context, the transition functions can be defined. They are applications between the two open systems \mathbb{R}^n , represented by functions as $q_{1i} = \varphi_{12i}(q_{1h})$ and $q_{2i} = \varphi_{21i}(q_{2h})$, useful to describe a change in coordinates between one map to another one.

Definition 3 ([11]). Two maps of dimension n , $\varphi_1 : U_1 \rightarrow \mathbb{R}^n$ and $\varphi_2 : U_2 \rightarrow \mathbb{R}^n$, are said C^k -compatible if $U_1 \cap U_2 = \emptyset$ or if, when $U_1 \cap U_2 \neq \emptyset$, the two following conditions occur:

1. The sets $O_1 = \varphi_1(U_1 \cap U_2)$ and $O_2 = \varphi_2(U_1 \cap U_2)$, image of the intersection of the two domain on the two maps, are open;
2. The transition function $\varphi_{12} : O_1 \rightarrow O_2$ and $\varphi_{21} : O_2 \rightarrow O_1$, defined as $\varphi_{12} = \varphi_2 \circ \varphi_1^{-1}$ and $\varphi_{21} = \varphi_1 \circ \varphi_2^{-1}$, with φ_1 and φ_2 of class C^k , are restricted to the intersection $U_1 \cap U_2$.

Definition 4 ([11]). On the set Q , a set of compatible maps is defined as $\mathcal{A} = \{\varphi_\alpha : U_\alpha \rightarrow \mathbb{R}^n; \alpha \in I\}$, with I set of indices with domains U_α , which are an overlap of Q . A set Q with atlas is said a differential variety of dimension n .

Comment 1. If the atlas has all the possible maps, it is said full or filled or maximum. A differential variety is a set with a maximum atlas.

Comment 2 ([11]). An atlas allows a topology, so a differential variety is also a topological space.

Definition 5 ([11]). A set of points $\{P_v, v \in B\}$ is said holonomic if its space of configurations Q has the structure of differentiable variety. Then, Q is said a variety of configurations. The dimension N of Q is said the number of freedom degrees of the system. The coordinates q_i related to every map of Q are said Lagrangian coordinates.

Comment 3 ([11]). $\forall v \in B, \exists \mathbf{r}_v : Q \rightarrow E_3$, i.e. there exists an application which assigns the position vector \mathbf{r}_v of the point P_v to any configuration of the system: known the coordinates q_i on Q the applications \mathbf{r}_v are vectorial functions $\mathbf{r}_v(q_i)$. Consequently, the velocity is

$$\dot{\mathbf{r}}_v = \sum_i \frac{\partial \mathbf{r}_v}{\partial q_i} \dot{q}_i.$$

Definition 6 ([11]). The motion act of a holonomic system is a set of vectors $(\mathbf{r}_v, \dot{\mathbf{r}}_v), v \in B$ such that:

$$\begin{cases} \mathbf{r}_v = \mathbf{r}_v(q_i) \\ \dot{\mathbf{r}}_v = \sum_i \frac{\partial \mathbf{r}_v}{\partial q_i} \dot{q}_i \end{cases} \quad (3)$$

Comment 4 ([11]). If Q is the configuration variety, then the set of the action acts is the tangent variety TQ ; indeed, the \dot{q}_i of the motion acts are the components of a vector tangent to Q on the coordinates q_i .

Definition 7 ([11]). A holonomic system is a system of points whose possible configurations in all times are a differentiable variety \bar{Q} of dimension $n + 1$, said space-time of the configurations, such that:

1. There exists a differentiable function $t : \bar{Q} \rightarrow \mathbb{R}$, which assigns to any configuration its time;
2. This application is such that $\forall t \in \mathbb{R}$ the set Q_t of all the possible configurations at the time t is a sub-variety of dimension n ;
3. There exists a differentiable variety Q of dimension n and a diffeomorphism $\varphi : \mathbb{R} \times Q \rightarrow \bar{Q}$, such that in any $i \in \mathbb{R}$ it generates a diffeomorphism $\varphi_i : Q \rightarrow Q_i : q \mapsto \varphi(t, q)$ between the variety Q and the variety Q_i .

The integer n is the number of degrees of freedom, and the variety Q is the reference configuration variety.

A holonomic system is made of constrained or free points. In dynamics, the action of the constraint is a force of reaction, called the constraint reaction, on which constitutive conditions must be imposed.

The smooth constraint is represented by the orthogonality between the constraint reaction and the constraint itself. For a holonomic system, for a forces configuration and system \mathbf{F}_v , applied to every motion act related to an assigned configuration, it corresponds to a power $W = \sum_v \mathbf{F}_v \cdot \dot{\mathbf{r}}_v$ of the forces; if the forces system is:

1. An active force system \mathbf{F}_{av} , then force laws related to positions and velocities are imposed, obtaining the consequent virtual power of the active forces $W_a^{(v)}$
2. A virtual motion acts with the constraint reaction system \mathbf{F}_{rv} , then a virtual power of the reactive forces W_r is considered.

Thus, it follows the definition:

Definition 8 ([11]). A holonomic system is perfect, or with perfect constraint, if the virtual power of the reactive forces is zero, for all virtual motion acts.

The virtual power of the active forces is a linear form of the components δq_i , whose coefficients are defined as Lagrangian forces or Lagrangian components of the active forces:

$$W_a^{(v)} = \sum_v \mathbf{F}_{av} \cdot \delta \mathbf{r}_v = \sum_v \mathbf{F}_{av} \cdot \sum_i \frac{\partial \mathbf{r}_v}{\partial q_i} \delta q_i = \sum_i \varphi_i \delta q_i \quad (4)$$

from which

$$\varphi_i = \sum_v \mathbf{F}_{av} \cdot \frac{\partial \mathbf{r}_v}{\partial q_i} \quad (5)$$

If the active forces are functions of the positions and of the velocities, then the Lagrangian forces are $\varphi = \varphi(\mathbf{q}, \dot{\mathbf{q}}, t)$.

Definition 9 ([11]). The dynamic state of a mechanical system is the time distribution of the positions, velocities, and accelerations of the points of the system.

A virtual power $W_m^{(v)}$ of the mass forces, named inertial forces, too, is associated with each dynamic state. The inertial forces are defined by the Newton Law

$$\mathbf{F}_{mv} = -m_v \mathbf{a}_v$$

The virtual power of the inertial forces is a linear form of the components δq_i of the virtual motion act, too:

$$W_m^{(v)} = \sum_v \mathbf{F}_{mv} \cdot \delta \mathbf{r}_v = - \sum_v m_v \mathbf{a}_v \cdot \sum_i \frac{\partial \mathbf{r}_v}{\partial q_i} \delta q_i = \sum_i \tau_i \delta q_i \quad (6)$$

from which it follows:

$$\tau_i = - \sum_v m_v \mathbf{a}_v \cdot \frac{\partial \mathbf{r}_v}{\partial q_i} \quad (7)$$

Statement 1 ([11] - Lagrange-D'Alembert Principle). In any dynamic state of a system with perfect constraints, for all virtual motion acts, the sum of the virtual powers of the active forces and the inertial forces equals zero:

$$W_a^{(v)} + W_m^{(v)} = 0 \quad (8)$$

A system (Q, \mathcal{L}) is said Lagrangian, if it is a differential variety Q of dimension n , said configuration variety, with an associated real function $\mathcal{L} : TQ \times \mathbb{R} \rightarrow \mathbb{R}$. If the system is time-independent the Lagrangian is a function

$$\mathcal{L} : TQ \rightarrow \mathbb{R}$$

The Lagrangian dynamics is the set of curves expressed by the first order system of $2n$ differentiable equations [11]:

$$\begin{cases} \dot{q}_i = \frac{dq_i}{dt} \\ \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right) - \frac{\partial \mathcal{L}}{\partial q_i} \end{cases} \quad (9)$$

where the (9)₂ equations are the Euler-Lagrange ones.

For the holonomic systems, the intrinsic properties of the Euler-Lagrange equations, i.e., the independence of the Lagrangian coordinates chosen, is the consequence of the application of the Lagrange-D'Alembert principle to a Lagrangian equation system.

A functional is an application $\phi : \Omega \rightarrow \mathbb{R}$ such that it corresponds to a real number for all n -tupla of functions. A functional is differentiable in a point $q_i(t) \in \Omega$ if for all the chooses of the growth, said variations, $\delta q_i(t) \in \Omega$ there exists the following relation [11]:

$$\phi(q_i + \delta q_i) = \phi(q_i) + \delta \phi(q_i, \delta q_i) + \mathcal{R} \quad (10)$$

where $\delta \phi$ is a linear functional of δq_i and \mathcal{R} is a functional of upper order in the same increases.

Definition 10 ([11]). A variation $\delta q_i(t)$ is said end fixed if:

$$\delta q_i(t_1) = \delta q_i(t_2) = 0 \quad (11)$$

Definition 11 ([11]). The action is defined as:

$$\mathcal{A} = \int_{t_1}^{t_2} \mathcal{L}(t, q_i(t), \dot{q}_i) dt \quad (12)$$

Theorem 1 ([12] - Least Action Principle). The function $q_i(t)$, for which $\delta \mathcal{A} = 0$ for all end fixed variations, are only the solutions of the differential system (9), where the Lagrangian is defined up to a function of the coordinates and time.

A general approach to mechanical systems can be developed by using the least action principle, also named Hamilton principle, for which the mechanical system is described using a Lagrangian function $\mathcal{L}(\mathbf{q}; \dot{\mathbf{q}}, t)$ from which the action can be obtained [12]:

$$\mathcal{A} = \int_{t_1}^{t_2} \mathcal{L}(\mathbf{q}; \dot{\mathbf{q}}, t) \quad (13)$$

The Hamilton principle states that the motion of a system follows the path $\mathbf{q}(t)$ for which the action is minimum:

$$\delta \mathcal{A} = \delta \int_{t_1}^{t_2} \mathcal{L}(\mathbf{q}; \dot{\mathbf{q}}, t) = 0 \quad (14)$$

The proof of this relation can be obtained starting from the hypothesis that the least value of the action is $\mathbf{q}(t)$, and a small variation $\delta \mathbf{q}$ around it, is considered. Then for

$$\mathbf{q}(t) + \delta \mathbf{q}(t) \quad (15)$$

the action S increases [12], but for $t = t_1$ and $t = t_2$ the relation (15) must have the fixed values $\mathbf{q}(t_1) = \mathbf{q}_1$ and $\mathbf{q}(t_2) = \mathbf{q}_2$; this statement represent fundamental condition for the Hamilton principle [12]:

$$\delta \mathbf{q}(t_1) = \delta \mathbf{q}(t_2) = 0 \quad (16)$$

A consequence of the least action principle is the Lagrange differential equations:

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial q_i} = 0 \quad i \in [1, n] \quad (17)$$

Non-holonomic constraints

A free point, from any initial position P_0 , at the initial time t_0 , can move of an elementary displacement $dP = \mathbf{v}dt$; for a constrained point, these displacements are confined due to the constraint [13]. A holonomic system in an initial configuration at the time t_0 , can have a transition to another configuration at the time $t_0 + dt$, infinitely near to the initial one [13].

Definition 12 ([13]). A possible displacement at the time t , starting from a configuration C , is any infinitesimal displacement of a holonomic system, which allows it to have a transition from the configuration C at the time t to a new configuration C' at the time $t + dt$:

$$P_i = P_i(\mathbf{q}; t) \mapsto P_i + dP_i = P_i(\mathbf{q} + d\mathbf{q}; t + dt)$$

from which the possible displacement are the n equations:

$$dP_i = \sum_k \frac{\partial P_i}{\partial q_k} dq_k + \frac{\partial P_i}{\partial t} dt = \nabla_{\mathbf{q}} P_i \cdot d\mathbf{q} + \frac{\partial P_i}{\partial t} dt \quad (18)$$

If the virtual displacement is coupled with the holonomic constraints Eqs. (1), related to the displacements themselves, represented by the l equations, it follows:

$$df_j = \sum_k \frac{\partial f_j}{\partial q_k} dq_k + \frac{\partial f_j}{\partial t} dt = \nabla_{\mathbf{q}} f_j \cdot d\mathbf{q} + \frac{\partial f_j}{\partial t} dt = 0 \quad (19)$$

and only $n - l$ free Lagrangian coordinates can be obtained. Dividing for dt the non-holonomic constraint relation can be obtained (2):

$$\frac{df_j}{dt} = \sum_k \frac{\partial f_j}{\partial q_k} \dot{q}_k + \frac{\partial f_j}{\partial t} = \nabla_{\mathbf{q}} f_j \cdot \dot{\mathbf{q}} + \frac{\partial f_j}{\partial t} = \sum_k a_{jk} \dot{q}_k + b_j = (\mathbf{a} \cdot \dot{\mathbf{q}} + b)_j = 0$$

(20)

It is a restrain in the motion.

So, the displacement are limited, and virtual displacements must be introduced:

Definition 13 ([13]). A virtual displacement is any hypothetical displacement that allows the system to have a transition from a configuration C to another infinitesimal near one C' , allowed by the constraints at the same time.

Consequently, for the non-holonomic constraints $dt = 0$, and the relation (20) becomes:

$$\nabla_{\mathbf{q}} f_j \cdot d\mathbf{q} + \frac{\partial f_j}{\partial t} dt = 0 \Rightarrow \mathbf{a} \cdot \delta \mathbf{q} = 0 \quad (21)$$

The live force is the value of the kinetic energy, and the following theorem can be introduced:

Theorem 2 ([14] - Theorem of Live Forces or of König). *The live force of any system in motion is the sum of the live force of the centre of mass, and the one of the motion in relation to the centre of mass.*

Volterra pointed out that the Lagrangian is an explicit function of $\dot{\mathbf{q}}$ [14].

Results

Non-holonomic systems, a term coined by Heinrich Rudolf Hertz (1857–1894) in 1894, are mechanical systems with constraints on their velocity that are not derivable from position constraints [9]. The non-holonomic constraint is non-integrable systems.

There are some differences between non-holonomic and Hamiltonian or Lagrangian systems, e.g. [9]:

- Non-holonomic systems arise from the Lagrange–d'Alembert principle and not from Hamilton's principle;
- Energy is always preserved, while momentum is not always preserved;
- Their volume in the phase space may not be preserved.

The equations of motion of a non-holonomic system in the form of the Euler–Lagrange equations, with the correction obtained by introducing some additional terms related to the constraints, but without Lagrange multipliers, when some of the configuration variables are cyclic, was obtained in 1895 by Sergej Alekseevič Čaplygin (1869–1942), who also realised the importance of an invariant measure in non-holonomic dynamics [9].

A fundamental question on the non-validity of the principle of least action for non-holonomic constraints, highlighted by Flannery [7], is suggested based on the previous definitions and theorems. In this paper, a possible response [15,16] to this question is proposed.

The basis of the least action principle is the evaluation of the variations under the hypothesis of the fix ends (Eq. (11)) [17].

For non-holonomic constraints (20) and (21), at least one of the virtual displacements can be written as a linear combination of the others; i.e.,

$$\delta q_i(t) = a_i^{-1} \sum_j a_{ij} \delta q_j \quad (22)$$

so the relations (20) e (21), fundamental for the validity of the least action principle, are not satisfied.

Consequently, for non-holonomic constraints, the fundamental conditions for using the least action principle are not verified, proving that for a general non-holonomic constraint, the principle of least action cannot be used. An alternative approach from thermodynamics is also suggested.

Discussion and conclusions

The proposed proof limits the use of the principle of least action to the holonomic and linear non-holonomic constraints [7]. But, it is important to find an alternative approach for generic non-holonomic systems. To do so, some considerations can be introduced from thermodynamics, particularly regarding the second law.

A thermodynamic system is a physical system which interacts with its environment by exchanging heat and work [18]. For such a system, it is possible to write the kinetic energy theorem in the following form [19–22]:

$$\delta W_{es} + \delta W_{fe} + \delta W_i = dE_k \quad (23)$$

where δ represents the pathway-dependent differential, W_{es} is the work done by external forces on the border of the system, W_{fe} is the work lost due to external irreversibility, E_k is the kinetic energy of the system, and W_i is the internal work, such that:

$$\delta W_i = \delta W_i^{rev} - \delta W_{fi} \quad (24)$$

where rev indicates the reversible (ideal) internal work and W_{fi} depicts the work lost due to internal irreversibility. Considering the relation [19,20,22]:

$$\delta W_{se} + \delta W_{es} + \delta W_{fe} = 0 \quad (25)$$

where W_{se} is the work by the internal forces on the system's border towards the outside of the system. As a consequence of this approach, the first law of thermodynamics appears in the following form:

$$\delta Q - \delta W_{se} = dU + dE_k \quad (26)$$

Now, defining the Lagrangian as [11,12]:

$$\mathcal{L} = E_k - E_p \quad (27)$$

where $E_p = W_i + W_{es}$ is the potential energy, it follows:

$$\mathcal{L} = E_k - (W_i + W_{es}) = W_{fe} \quad (28)$$

Now, we consider the Gouy–Stodola theorem [23,24]:

$$W_{fe} = -T_0 \int_0^\tau \Sigma \cdot dt \quad (29)$$

where T_0 is the environmental temperature, Σ is the entropy generation rate, and t is the time. Considering the duration of a process τ , i.e., the time in which a process occurs, and the mean value of the entropy generation rate $\bar{\Sigma}$, it is possible to obtain the entropy generation, S_g , for any real process by using an engineering thermodynamic approach, as follows [25,26]:

$$S_g = \bar{\Sigma} \cdot \tau \quad (30)$$

Consequently, the Lagrangian results [23,26]:

$$\mathcal{L} = -T_0 S_g \quad (31)$$

and the action \mathcal{A} results [23,26]:

$$\mathcal{A} = -T_0 \int S_g dt \quad (32)$$

This last relation is very interesting because the entropy generation results always integrable for a real process, as usually done in engineering thermodynamics, independently on the formal expression of the displacements, obtaining [23,26]:

$$\mathcal{A} = -T_0 \bar{S}_g \tau \quad (33)$$

consequently, the least action can be used by evaluating the maximum entropy generation, which is related only to dissipation. In this way, the analysis of the motion for non-holonomic systems becomes the analysis of the dissipation during the motion.

These considerations represent a starting point in the analysis of non-holonomic constraints, proposing a thermodynamic viewpoint,

which analytically confirms, on the bases of the first and second law of thermodynamics, the considerations highlighted in Ref. [27].

In this context, in 2019, Mahulikar et al. [28] developed a non-equilibrium thermodynamic study analysing the Fluctuation Theorem and Principle of Least Action implication for dissipative systems. They pointed out that the Principle of Maximum Entropy Production acts like the Principle of Least Action for dissipative systems. Moreover, they introduced the Thermodynamic Fusion Theorem for addressing the role of fluctuations in entropy production, identifying the entropy fluctuation as the least action path, which maximises the time-averaged entropy production in a dissipative system. The validation of their results was proven for the analysis of the entropy fluctuations in Rayleigh–Taylor flow instability [29].

In conclusion, in this paper, we have combined our previous results [15,16,25,26,30,31] with the results of Mahulikar et al. [28] obtaining a general approach to the use of least action principle to non-holonomic constraints, pointing out that Principle of Maximum Entropy Production is a generalisation of the Principle of Least Action for real systems.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article

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