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An entropy-based evaluation of contact forces in continuum mechanics of elastic structures

Zhaocheng Xuan [a,*], Panayiotis Papadopoulos [b], Jianyu Li [c], Lili Zhang [a]

[a] Department of Computer Science, Tianjin University of Technology and Education, Tianjin 300222, China
[b] Department of Mechanical Engineering, University of California, Berkeley, CA 94720-1740, USA
[c] Department of Mechanical Engineering, Tianjin University of Science and Technology, Tianjin 300222, China

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ABSTRACT

The maximum entropy principle has proved to be a versatile tool for solving problems in many fields. In this paper, we extend entropy and its use in statistical physics to evaluate contact forces in the continuum mechanics of elastic structures. Each potential contact node of an elastic structure discretized by finite elements along with the normalized contact force on the node is considered as a system and all potential contact nodes together with their normalized contact forces are considered as a canonical ensemble, with the normalized contact force of each node representing the microstate of the node. The product of non-penetration conditions for potential contact nodes and the normalized nodal contact forces then act as an expectation that its value will be zero, and maximizing the entropy under the constraints of the expectation and the minimum potential energy principle results in an explicit probability distribution for the normalized contact forces that shows the relation between contact forces and displacements in a formulation similar to the formulation for particles occupying microstates in statistical physics. Moreover, an iterative procedure that solves a series of isolated systems to find the contact forces is presented, with a novel termination condition. Finally, some examples are examined to verify the correctness and efficiency of the procedure.

1. Introduction

Entropy is one of the core concepts in statistical physics and information theory [1–4], and the parallelism between the two subjects goes beyond replacing one name with another, as each gives us a new way of thinking about the other. The concept of entropy has been used in various fields of science and engineering and has received much attention in problems aimed at determining the disorder, possibility, or uncertainty in a physical ensemble. Entropy is a versatile tool for solving problems in different fields – for example, it has been used to solve granular materials problems using microstate quantity to determine the macrostate quantity [5–9] and has also been used to solve moment problems in solid-state physics [10,11], geophysical applications [12–14], econometrics [15], and transport planning [16,17].

At the same time, entropy is also thought of as merely a very useful formalism, that is, a convenient means for understanding and representing physical principles in mathematical terms. In solving optimization problems, Li was the first to think of the activity or inactivity of constraints as their possibility, and used the maximum entropy principle to change the multi-constraints problem into a single constraint problem [18,19]. Entropy has also been added to the objective function in optimization problems, where it plays the role of a penalty function to accelerate the process of optimization [20].

Although entropy has been used in many fields, to the best of our knowledge, there is very little work that uses entropy in solving contact forces, except in granular material, which we believe is the largest scale material for which entropy has been related to contact forces. Thus the question arises: Can entropy be used to solve contact forces in the continuum mechanics of elastic bodies? The contact mechanics of continuum elasticity is foundational to the field of mechanical engineering; it provides necessary information for the safe and energy efficient design of technical systems and for the study of tribology and indentation hardness. It is one type of highly nonlinear mechanics and studies the deformation of solids that touch each other at one point or more. Central ingredients of contact mechanics include the pressures and adhesion acting perpendicular to the contacting bodies' surfaces, the normal direction, and the frictional stresses acting tangentially between the surfaces [21].

* Corresponding author.
E-mail address: xuanzc@tute.edu.cn (Z. Xuan).

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Numerical methods have proved to be the most efficient means for solving problems in contact mechanics [22,23]. In this paper, we provide an alternative to numerical methods, namely, an entropy-based procedure, to interpret and solve the contact forces of elastic bodies, focusing mainly on the normal direction, i.e., on frictionless contact mechanics. The elastic bodies discretized by finite elements are considered as an environment, each potential contact node (or node pair, *sic passim*) along with the normalized contact force on it is considered as a system, and all potential contact nodes along with their normalized contact forces are considered as a canonical ensemble, with the normalized contact forces representing the microstates of the contact nodes. Using the maximum entropy principle, the relationship between the normalized contact forces and the displacements can be constructed. The displacements of the elastic body can be treated as the *temperature* source for the non-isolated environment. Given this formulation, we present an iterative procedure that can then solve a series of isolated ensembles for finding the contact forces, with the monotonicity of the potential energy used as a termination condition.

The rest of this paper is organized as follows. In the next section, a short introduction to entropy formulation in statistical physics is presented and entropy-based formulations for contact forces are derived. Section 3 presents an iterative procedure for the contact forces along with a detailed interpretation of the maximum entropy principle and the minimum potential energy principle. In Section 4, some examples are analyzed to verify the correctness and performance of the iterative procedure, and the final section presents the papers conclusions.

2. Entropy-based formulation for contact forces

2.1. Entropy in statistical physics

Let us define an ensemble as consisting of m systems or particles, where the probability of system i occupying a microstate is p_i. A canonical ensemble is an ensemble defined by the probability $\mathbf{p}=\{p_1,p_2,\ldots,p_m\}^T$ that characterizes the microstates of a system in equilibrium with an environment at temperature T. Maximizing the Gibbs entropy $S=-\kappa\mathbf{p}^T\ln\mathbf{p}$ subject to the normalization condition $\mathbf{1}^T\mathbf{p}=1$ and an expectation value of energy $\langle E\rangle=\mathbf{e}^T\mathbf{p}$ is equivalent to finding the stationery condition of the following Lagrangian function:

$$L(\mathbf{p},\gamma,\delta)=-\kappa\mathbf{p}^T\ln\mathbf{p}+\gamma(\mathbf{e}^T\mathbf{p}-\langle E\rangle)+\delta(\mathbf{1}^T\mathbf{p}-1), \tag{1}$$

where κ is a coefficient related to the ensemble, γ and δ are Lagrange multipliers corresponding to the two constraints, namely, the normalization condition and the expectation, respectively, and $\mathbf{e}=\{e_1,e_2,\ldots,e_m\}^T$ is the energy of the particles. In this paper, we follow the convention of denoting matrices or vectors with bold letters and logarithmic functions or exponential functions in compact forms, e.g., $\mathbf{1}=\{1,\ldots,1\}^T$, $\ln\mathbf{p}=\{\ln p_1,\ldots,\ln p_m\}^T$, $\exp(\mathbf{p})=\{\exp(p_1),\ldots,\exp(p_m)\}^T$. Letting the differential of Eq. (1) with respect to $\mathbf{p}$ be zero, that is,

$$-\kappa\ln\mathbf{p}-\kappa\mathbf{1}+\gamma\mathbf{e}+\delta\mathbf{1}=\mathbf{0}, \tag{2}$$

we can express $\mathbf{p}$ in terms of $\mathbf{e}$ as follows:

$$\mathbf{p}=\exp\left(\frac{\delta}{\kappa}\mathbf{1}-\mathbf{1}+\frac{\gamma}{\kappa}\mathbf{e}\right)=\exp\left(\frac{\delta}{\kappa}-1\right)\exp\left(\frac{\gamma}{\kappa}\mathbf{e}\right). \tag{3}$$

Using the normalization condition $\mathbf{1}^T\mathbf{p}=1$, we then obtain

$$\mathbf{p}=\frac{\exp\left(\frac{\gamma}{\kappa}\mathbf{e}\right)}{Z}, \tag{4}$$

where Z is the system partition function, a sum over the microstates of the system,

$$Z=\mathbf{1}^T\exp\left(\frac{\gamma}{\kappa}\mathbf{e}\right). \tag{5}$$

The relationship between the entropy S, system energy E, and temperature T can be captured as $\frac{1}{T}=\frac{\partial S}{\partial E}$, and so for this case of a non-isolated system, we have

$$\frac{1}{T}=\frac{\partial S}{\partial\langle E\rangle}. \tag{6}$$

Now let us use it to eliminate the Lagrange multiplier γ. Substituting $\ln\mathbf{p}=\frac{\gamma}{\kappa}\mathbf{e}-\ln Z\mathbf{1}$ into the entropy S, we have

$$S=-\gamma\langle E\rangle+\kappa\ln Z, \tag{7}$$

and given

$$\frac{\partial\ln Z}{\partial\gamma}=\frac{1}{\kappa Z}\mathbf{e}^T\exp\left(\frac{\gamma}{\kappa}\mathbf{e}\right)=\frac{1}{\kappa}\mathbf{p}^T\mathbf{e}=\frac{1}{\kappa}\langle E\rangle, \tag{8}$$

the following equation holds:

$$\frac{\partial S}{\partial\langle E\rangle}=-\gamma-\left(\langle E\rangle-\kappa\frac{\partial\ln Z}{\partial\gamma}\right)\frac{\partial\gamma}{\partial\langle E\rangle}=-\gamma. \tag{9}$$

Therefore, the relationship between $\mathbf{p}$, E and T is as follows:

$$\mathbf{p}=\frac{\exp\left(-\frac{1}{\kappa T}\mathbf{e}\right)}{\mathbf{1}^T\exp\left(-\frac{1}{\kappa T}\mathbf{e}\right)}. \tag{10}$$

The probability is obtained by maximizing the entropy for a system, and it has been proved that the entropy for a system is simply $\frac{1}{m}$ of the entropy of the ensemble, so maximizing the entropy of the ensemble will also produce the same results as Eq. (10). More details on entropy in statistical physics can be found in [4] and its references.

2.2. Entropy in contact mechanics

Let us consider an elastic structure of two bodies coming into contact; see Fig. 1. The boundary of the elastic bodies consists of the displacement boundary Γ_v, the external loads boundary Γ_t, and the potential contact boundary Γ_c. The elastic bodies are discretized by finite elements, and the finite element nodes are separated into two groups: one includes the potential contact nodes on the potential contact boundary, and the other includes the nodes on the rest of the body. We consider the contact part as a canonical ensemble, as in statistical physics. Table 1 presents a comparison of entropy in statistical physics and in contact mechanics.

Analogously to the derivation in Section 2.1, we write the entropy in the form $S=-\rho\boldsymbol{\lambda}^T\ln\boldsymbol{\lambda}$, and the Lagrangian function for the elastic contact problem is

$$L(\boldsymbol{\lambda},\alpha,\beta)=-\rho\boldsymbol{\lambda}^T\ln\boldsymbol{\lambda}+\alpha\boldsymbol{\lambda}^Td(\mathbf{u})+\beta(\mathbf{1}^T\boldsymbol{\lambda}-1), \tag{11}$$

where α and β are Lagrange multipliers, $d(\mathbf{u})$ is the function of displacement related to the potential contact nodes, and $\boldsymbol{\lambda}$ is the

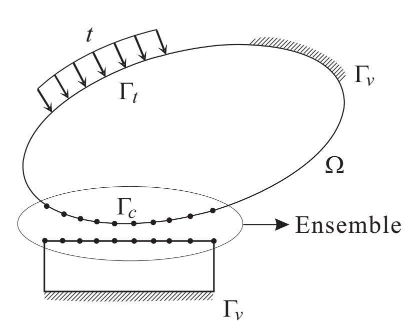

Fig. 1. An elastic body coming into contact with a foundation.