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# Identifying second-gradient continuum models in particle-based materials with pairwise interactions using acoustic tensor methodology.

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## Abstract

This paper discusses wave propagation in unbounded particle-based materials described by a second-gradient continuum model, recently introduced by the authors, to provide an identification technique. The term *particle-based* materials denotes materials modeled as assemblies of particles, disregarding typical *granular* material properties such as contact topology, granulometry, grain sizes, and shapes. This work introduces a center-symmetric second-gradient continuum resulting from pairwise interactions. The corresponding Euler-Lagrange equations (equilibrium equations) are derived using the least action principle. This approach unveils non-classical interactions within subdomains. A novel, symmetric, and positive-definite acoustic tensor is constructed, allowing for an exploration of wave propagation through perturbation techniques. The properties of this acoustic tensor enable the extension of an identification procedure from Cauchy (classical) elasticity to the proposed second-gradient continuum model. Potential applications concern polymers, composite materials, and liquid crystals.

**Keywords:** Nonlocal elasticity, second-gradient continuum, acoustic tensor, identification, bulk waves

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## 1. Introduction

This theoretical paper aims to propose a methodology for experimentally identifying the constitutive tensors involved in a second-gradient model applicable to particle-based materials with pairwise interactions. The proposed methodology devoted to experimental identification uses the properties of an acoustic tensor obtained within the framework of the considered second-gradient model. This work does not address numerical aspects; for information on this topic, we recommend consulting the cited references [1, 2].

With particle-based materials, we refer to materials that can be modeled as an assembly of point materials, or particles. While the terms particle-based and *granular* are often used interchangeably in the literature, they are not synonymous. In the context of particle-based materials, factors such as the topology of contacts between adjacent grains, granulometry, grain sizes, and shapes are not deemed to have a significant impact on the modeling and are therefore disregarded. Since polymers, composite materials, and liquid crystals can be regarded as particle-based materials, the development of sophisticated models for particle-based materials is of fundamental importance from a practical standpoint. To further emphasize the practical applications, it is noteworthy that among all the candidate materials, colloidal crystals emerge as a significant class of particle-based materials. They find extensive applications, for instance in materials sciences [3, 4], biology [5], optical materials [6], and 3D printing technology [7, 8].

In recent years, there has been significant advancement in the development of continuum models tailored to capture the mesoscale behavior of particle-based materials. Examples include the application of micropolar continuum theories [9, 10, 11, 12, 13, 14], micromorphic continuum theories [15, 16, 17, 18], integral nonlocal continuum theories [19, 20, 21], and gradient-type nonlocal continuum theories [22, 23, 24, 25, 26, 27, 28]. These continuum models have also been named continuum-molecular formulations in [29] and continuum particle models in [30]. Additional continuum-type formulations, proposing pairwise interactions, have been developed and referred to as continuum-molecular formulations in [29] and continuum particle models in [30]. The collection of all these models is referred to as *generalized continua* [31]. Among generalized continua, second-gradient continuum models have gained substantial attention for their capability to describe size effects without introducing rotational degrees of freedom [32, 33, 34].

For engineering purposes, the primary challenge in using generalized continua, and then second-gradient continua, lies in accurately identifying constitutive parameters. The identification problem is typically addressed in the literature by constructing generalized continua as homogenized models of microscopic Cauchy (classical) materials. In this way, only parameters related to Cauchy elasticity need to be identified for applying generalized continua. Construction of a homogeneous Cosserat continuum starting from a micro-heterogeneous Boltzmann continuum has

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been proposed in [35]. The general case of a micromorphic continuum has been addressed in [36, 37], and works related to the second-gradient continua can be found in [38, 39, 40, 41]. In most cases, homogenization procedures require the definition of a representative volume element and consideration concerning the extended Hill-Mandel condition [42].

As previously stated, this paper is the continuation of [1, 2]. In [1], we introduced a second-order tensor to describe nonlocal pairwise interactions that would correspond to the Green-Lagrange tensor [43, 44] in a nonlocal framework. This second-order tensor allows us to obtain a higher-order nonlocal continuum model that includes the Piola peridynamics and the Eringen nonlocal elasticity. It should be noted that the term Piola peridynamics refers to the peridynamics approach developed by Piola, which differs from the commonly adopted approaches and is closely related to bond-based peridynamics [45]. In [2], we further refined the novel higher-order nonlocal continuum model and we incorporated random fields [46, 47, 48, 49], constructed using the maximum entropy principle [50, 51].

The present paper is organized as follows. In Section 2, we investigate more deeply the novel higher-order nonlocal continuum model for particle-based materials, obtaining a center-symmetric second-gradient continuum resulting from pairwise particle interactions. This model positions itself between integral and gradient-type nonlocal continua [52]. The Euler-Lagrange equations (equilibrium equations) are derived using the least action principle. In Section 3, we construct a novel acoustic tensor that is symmetric and positive definite. In Section 4, the perturbation technique is then applied to investigate the impact of second-gradient terms on wave perturbation within the framework of the proposed model. The relationship between phase and group velocities is investigated. Moving on to Section 5, the properties of the introduced acoustic tensor allow us to extend the identification procedure proposed in [53] for Cauchy continua to the proposed center-symmetric second-gradient continuum. Thus, we show that, for any class of symmetry, the non-classical constitutive tensors and interaction length of the proposed center-symmetric second-gradient model can be extracted from experimentally measured propagation velocities of bulk waves. An application of the identification approach is not addressed here, as it has already been illustrated in the case of Cauchy continua in [53].

## Notation

Any vector in  $\mathbb{R}^3$  is identified to the column matrix of its components on the canonical basis of  $\mathbb{R}^3$ . Any tensor of any order will be represented by its components on the canonical basis. The components of a fourth-order tensor  $\mathbf{x}$  will be denoted by  $x_{ijkl}$ . In particular, any second-order tensor will be represented with the matrix of its components. In addition, the classical convention of summation on repeated indices is used.

A lowercase letter such as  $x$ ,  $y$  or  $z$  is a real variable except when used as an integer index as  $i$ ,  $j$ , etc.

A boldface lowercase letter such as  $\mathbf{x}$  or  $\boldsymbol{\xi}$  is a real vector and such as  $\mathbf{c}$  or  $\boldsymbol{\lambda}$  is a tensor.

A boldface lowercase letter between brackets, such as  $[\mathbf{x}]$ ,  $[\mathbf{y}]$ , or  $[\mathbf{z}]$ , is a real matrix. The entries of  $[\mathbf{x}]$  will be denoted by  $[\mathbf{x}]_{ij}$ .

$\langle \mathbf{x}, \mathbf{y} \rangle$ : standard inner product in Euclidean space  $\mathbb{R}^n$ .

$\|\mathbf{x}\|$ : Euclidean norm in  $\mathbb{R}^n$  equal to  $\langle \mathbf{x}, \mathbf{x} \rangle^{1/2}$ .

$[\mathbf{x}]^T$ : transpose of the matrix  $[\mathbf{x}]$ .

$[\mathbf{I}]$ : identity matrix.

$\mathbb{M}_n$ : ensemble of  $n \times n$  real matrices.

$\mathbb{M}_n^S$ : subset of  $\mathbb{M}_n$  of symmetric matrices.

$\mathbb{M}_n^+$ : subset of  $\mathbb{M}_n^S$  of positive definite matrices.

$\mathbb{M}_{n \text{diag}}^+$ : subset of  $\mathbb{M}_n^+$  of diagonal matrices.

$\mathbb{T}_4$ : ensemble of 4-th order real tensors  $\mathbb{t}_{ijkl}$ .

$\mathbb{T}_4^S$ : subset of  $\mathbb{T}_4$  of symmetric tensors such that  $\mathbb{t}_{ijkl} = \mathbb{t}_{jikl} = \mathbb{t}_{ijlk} = \mathbb{t}_{klij}$ .

$\mathbb{T}_4^+$ : subset of  $\mathbb{T}_4^S$  of positive definite tensors.

$C^N(\Omega)$ : set of real functions defined on  $\Omega$ , which are  $N$  times continuously differentiable.

The summation over repeated Latin indices is used.

## 2. Defining the Second-Gradient Continuum Theory for Particle-Based Materials

This section summarizes the results presented in [1, 2] concerning an  $N$ -th order nonlocal elasticity continuum model and its adaptation to the second-gradient case. We are limiting the presentation to the second-gradient case instead of  $N$ -th gradient one to simplify the writing and the reading. The extension to the  $N$ -th gradient case does not introduce any theoretical difficulties but would require additional analyses concerning the definition and the properties of the acoustic tensor. In the first subsection, we introduce the kinematic aspects of the second-gradient case and the expressions for small deformations. The second subsection deals with the least action principle. Finally, in the third subsection, we derive from it the Euler-Lagrange equations (equilibrium equations).

### 2.1. Geometry definition

Let us consider a continuum body that occupies the open, bounded, and connected domain  $\Omega$ , with a Lipschitz-continuous boundary  $\partial\Omega$ , defining the reference configuration (see [44]). It is assumed that  $\partial\Omega$  contains edges and is written as  $\partial\Omega = \cup_k \partial\bar{\Omega}_k$ , where  $\partial\Omega_k$  is an open, bounded, and connected domain, and  $\partial\bar{\Omega}_k = \partial\Omega_k \cup \partial\partial\Omega_k$ . We define the Lipschitz-continuous boundary  $\partial\partial\Omega$  as  $\cup_k \partial\partial\Omega_k = \partial\partial\Omega$ , which is the union, with edge repetitions, of the edges  $\partial\partial\Omega_k$ . We will denote by  $\int_{\partial\partial\Omega} = \sum_k \int_{\partial\partial\Omega_k}$ . Let  $\mathbf{x}$  be the generic point of  $\Omega$ . Let  $d\mathbf{x}$ ,  $ds$ , and  $d\ell$  be the volume, surface, and length elements. Therefore, the  $ds$ -measure of  $\partial\partial\Omega$  is zero. For  $\mathbf{x}$  in  $\partial\Omega_k$ ,  $\mathbf{n}(\mathbf{x})$  denotes the outward-pointing unit normal of  $\partial\Omega_k$ . For  $\mathbf{x}$  in  $\partial\partial\Omega_k$ ,  $\mathbf{v}(\mathbf{x})$  denotes the outward-pointing unit normal of  $\partial\partial\Omega_k$ . Let  $\{\xi_1, \xi_2, \xi_3\}$  be the canonical basis of  $\mathbb{R}^3$ . Both reference and deformed configurations are referred to the Cartesian coordinate system  $(O, \xi_1, \xi_2, \xi_3)$ .

### 2.2. Kinematic aspects

**Definition 1 (Placement function and its regularity properties).** Let  $(\mathbf{x}, t) \mapsto \mathbf{r}(\mathbf{x}, t)$ , with  $t \in \mathbb{R}$ , be the placement function defining the motion of  $\Omega$ , satisfying the following conditions.

- C.1 For any fixed instant  $t$  in  $\mathbb{R}$ ,  $\mathbf{x} \mapsto \mathbf{r}_t(\mathbf{x}) = \mathbf{r}(\mathbf{x}, t)$ , defined from  $\bar{\Omega}$  into  $\mathbb{R}^3$ , is assumed to be in  $C^2(\bar{\Omega})$ , injective except possibly on the boundary  $\partial\Omega$ , and orientation-preserving (see [44]).
- C.2 For any fixed  $\mathbf{x}$  in  $\Omega$ ,  $t \mapsto \mathbf{r}_\mathbf{x}(t) = \mathbf{r}(\mathbf{x}, t)$  has a first-order derivative  $t \mapsto d\mathbf{r}_\mathbf{x}(t)/dt$  in  $C^1(\mathbb{R})$  and a second-order derivative  $t \mapsto d^2\mathbf{r}_\mathbf{x}(t)/dt^2$  piecewise continuous in  $\mathbb{R}$  (see [54]).

**Hypothesis 1 (Nonlocal interaction between particles).** Let  $\mathbf{x}$  in  $\Omega$  and let  $\bar{\mathbf{x}}$  be another point in a neighborhood of  $\mathbf{x}$ . Let us assume a nonlocal interaction between particles at order  $O(\|\bar{\mathbf{x}} - \mathbf{x}\|^3)$ , allowing us to approximate  $\mathbf{r}$  at the point  $\bar{\mathbf{x}} \in \Omega$  using its truncated second-order Taylor expansion in the neighborhood of  $\mathbf{x} \in \Omega$ ,

$$r_i(\bar{\mathbf{x}}, t) = r_i(\mathbf{x}, t) + \frac{\partial r_i(\mathbf{x}, t)}{\partial x_j} (\bar{x}_j - x_j) + \frac{1}{2} \frac{\partial^2 r_i(\mathbf{x}, t)}{\partial x_j \partial x_k} (\bar{x}_j - x_j)(\bar{x}_k - x_k). \quad (1)$$

**Definition 2 (Kinematic tensors).** Let  $\mathbf{f}^{(1)}(\mathbf{x}, t)$  be the second-order tensor represented by the matrix  $[\mathbf{f}^{(1)}(\mathbf{x}, t)]$  such that

$$[\mathbf{f}^{(1)}(\mathbf{x}, t)]_{ij} = \frac{\partial r_i(\mathbf{x}, t)}{\partial x_j} \quad (2)$$

and let  $\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)$  be the second-order tensor represented by the matrix  $[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)]_{ij}$  such that

$$[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)]_{ij} = [\mathbf{f}^{(1)}(\mathbf{x}, t)]_{ij} + \frac{1}{2} \frac{\partial [\mathbf{f}^{(1)}(\mathbf{x}, t)]_{ij}}{\partial x_k} (\bar{x}_k - x_k). \quad (3)$$

Taking into account Eq. (2) and (3), Eq. (1) can be rewritten as

$$\mathbf{r}(\bar{\mathbf{x}}, t) = \mathbf{r}(\mathbf{x}, t) + [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)] (\bar{\mathbf{x}} - \mathbf{x}), \quad (4)$$

where  $\det[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)] > 0$  under the hypothesis of orientation-preserving deformations. Let us define the Cauchy-Green second-order tensor  $\mathbf{c}^{(1)}(\mathbf{x})$  represented by the matrix  $[\mathbf{c}^{(1)}(\mathbf{x})]$  in  $\mathbb{M}_3^+$  such that

$$[\mathbf{c}^{(1)}(\mathbf{x}, t)] = [\mathbf{f}^{(1)}(\mathbf{x}, t)]^T [\mathbf{f}^{(1)}(\mathbf{x}, t)], \quad (5)$$

the third-order tensor  $\mathbf{c}^{(12)}(\mathbf{x}, t)$ , and the fourth-order tensor  $\mathbf{c}^{(2)}(\mathbf{x}, t)$  whose components are

$$c_{pqj}^{(12)}(\mathbf{x}, t) = \frac{\partial [\mathbf{c}^{(1)}(\mathbf{x}, t)]_{pq}}{\partial x_j}, \quad c_{pqjk}^{(2)}(\mathbf{x}, t) = \frac{\partial [\mathbf{f}^{(1)}(\mathbf{x}, t)]_{ip}}{\partial x_j} \frac{\partial [\mathbf{f}^{(1)}(\mathbf{x}, t)]_{iq}}{\partial x_k}. \quad (6)$$

Let  $\mathbf{e}^{(1)}(\mathbf{x}, t)$ ,  $\mathbf{e}^{(12)}(\bar{\mathbf{x}}, \mathbf{x}, t)$ , and  $\mathbf{e}^{(2)}(\bar{\mathbf{x}}, \mathbf{x}, t)$  be the tensors represented by the matrices  $[\mathbf{e}^{(1)}(\mathbf{x}, t)]$ ,  $[\mathbf{e}^{(12)}(\bar{\mathbf{x}}, \mathbf{x}, t)]$ , and  $[\mathbf{e}^{(2)}(\bar{\mathbf{x}}, \mathbf{x}, t)]$  in  $\mathbb{M}_3^S$  such that

$$[\mathbf{e}^{(1)}(\mathbf{x}, t)] = \frac{1}{2}([\mathbf{c}^{(1)}(\mathbf{x}, t)] - [\mathbf{I}]), \quad (7)$$

$$[\mathbf{e}^{(12)}(\bar{\mathbf{x}}, \mathbf{x}, t)]_{pq} = \frac{1}{4}c_{pqj}^{(12)}(\mathbf{x}, t)(\bar{x}_j - x_j), \quad (8)$$

and

$$[\mathbf{e}^{(2)}(\bar{\mathbf{x}}, \mathbf{x}, t)]_{pq} = \frac{1}{8}c_{pqjk}^{(2)}(\mathbf{x}, t)(\bar{x}_j - x_j)(\bar{x}_k - x_k). \quad (9)$$

Let us define the tensor  $\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x}, t)$ , represented by the matrix  $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x}, t)]$  in  $\mathbb{M}_3^S$ , by

$$[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x}, t)] = \frac{1}{2}([\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)]^T [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)] - [\mathbf{I}]). \quad (10)$$

Using Eq. (3),  $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x}, t)]$  can be rewritten (See Appendix A) as

$$[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x}, t)] = [\mathbf{e}^{(1)}(\mathbf{x}, t)] + [\mathbf{e}^{(12)}(\bar{\mathbf{x}}, \mathbf{x}, t)] + [\mathbf{e}^{(2)}(\bar{\mathbf{x}}, \mathbf{x}, t)]. \quad (11)$$

**Remark 1.** From Eq. (4), considering the definition of the transpose operator, we obtain

$$\|\mathbf{r}(\bar{\mathbf{x}}, t) - \mathbf{r}(\mathbf{x}, t)\|^2 - \|\bar{\mathbf{x}} - \mathbf{x}\|^2 = \langle 2[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x}, t)](\bar{\mathbf{x}} - \mathbf{x}), (\bar{\mathbf{x}} - \mathbf{x}) \rangle. \quad (12)$$

Note that Eq. (12) is obtained using the definition of  $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x}, t)]$  and the fact that  $\|\mathbf{r}(\bar{\mathbf{x}}, t) - \mathbf{r}(\mathbf{x}, t)\|^2 - \|\bar{\mathbf{x}} - \mathbf{x}\|^2$  is equal to  $\langle [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)] \Delta \mathbf{x}, [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)] \Delta \mathbf{x} \rangle - \langle [\mathbf{I}] \Delta \mathbf{x}, \Delta \mathbf{x} \rangle$ . This expression, thanks to the definition of transpose, is also equal to  $\langle [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)]^T [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)] \Delta \mathbf{x}, \Delta \mathbf{x} \rangle - \langle [\mathbf{I}] \Delta \mathbf{x}, \Delta \mathbf{x} \rangle$ .

Tensor  $\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x}, t)$  characterizes the configuration change within the continuum due to the movement of  $\bar{\mathbf{x}}$  with respect to  $\mathbf{x}$  over time  $t$ . This tensor is the sum of three distinct deformation mechanisms through tensors  $\mathbf{e}^{(1)}(\mathbf{x}, t)$ ,  $\mathbf{e}^{(12)}(\bar{\mathbf{x}}, \mathbf{x}, t)$ , and  $\mathbf{e}^{(2)}(\bar{\mathbf{x}}, \mathbf{x}, t)$ . Tensors  $\mathbf{e}^{(1)}(\mathbf{x}, t)$ ,  $\mathbf{e}^{(12)}(\bar{\mathbf{x}}, \mathbf{x}, t)$ , and  $\mathbf{e}^{(2)}(\bar{\mathbf{x}}, \mathbf{x}, t)$  are obtained by fixing  $\mathbf{x}$  and expanding  $\mathbf{r}$  in the neighborhood of  $\mathbf{x}$ . Thus, they account for the effects of the movements of  $\bar{\mathbf{x}}$  with respect to  $\mathbf{x}$ . In contrast, to address the effects of the movements of  $\mathbf{x}$  with respect to  $\bar{\mathbf{x}}$ , we can use tensors  $\mathbf{e}^{(1)}(\bar{\mathbf{x}}, t)$ ,  $\mathbf{e}^{(12)}(\mathbf{x}, \bar{\mathbf{x}}, t)$ , and  $\mathbf{e}^{(2)}(\mathbf{x}, \bar{\mathbf{x}}, t)$  by switching the positions of  $\mathbf{x}$  and  $\bar{\mathbf{x}}$ . Consequently, within this kinematic framework, the nonlocal specific deformation energy is assumed to be symmetric in  $\mathbf{x}$  and  $\bar{\mathbf{x}}$ , dependent on  $\mathbf{e}^{(1)}(\mathbf{x}, t)$ ,  $\mathbf{e}^{(1)}(\bar{\mathbf{x}}, t)$ ,  $\mathbf{e}^{(12)}(\bar{\mathbf{x}}, \mathbf{x}, t)$ ,  $\mathbf{e}^{(12)}(\mathbf{x}, \bar{\mathbf{x}}, t)$ ,  $\mathbf{e}^{(2)}(\bar{\mathbf{x}}, \mathbf{x}, t)$ , and  $\mathbf{e}^{(2)}(\mathbf{x}, \bar{\mathbf{x}}, t)$ . Note that, in this manner, we take into account local and nonlocal deformation mechanisms associated with the change in distance between  $\bar{\mathbf{x}}$  and  $\mathbf{x}$ . Therefore, the resulting second-gradient model has to be considered based on pairwise particle interactions.

**Hypothesis 2 (Case of small deformations).** We add the hypothesis of small deformations and we assume that there are no rigid body displacements. Let  $\mathbf{u}$  be the displacement field such that  $\mathbf{r}(\mathbf{x}, t) = \mathbf{u}(\mathbf{x}, t) + \mathbf{x}$ . Let us define  $\boldsymbol{\epsilon}^{(1)}(\mathbf{x}, t)$  and  $\boldsymbol{\epsilon}^{(12)}(\bar{\mathbf{x}}, \mathbf{x}, t)$  as the approximation of  $\mathbf{e}^{(1)}(\mathbf{x}, t)$  and  $\mathbf{e}^{(12)}(\bar{\mathbf{x}}, \mathbf{x}, t)$  for small deformations,

$$[\boldsymbol{\epsilon}^{(1)}(\mathbf{x}, t)]_{pq} = \frac{1}{2} \left( \frac{\partial u_p(\mathbf{x}, t)}{\partial x_q} + \frac{\partial u_q(\mathbf{x}, t)}{\partial x_p} \right), \quad (13)$$

$$[\boldsymbol{\epsilon}^{(12)}(\bar{\mathbf{x}}, \mathbf{x}, t)]_{pq} = \frac{1}{4} \kappa_{pqj}^{(12)}(\mathbf{x}, t)(\bar{x}_j - x_j) \quad , \quad \kappa_{pqj}^{(12)} = 2 \frac{\partial [\boldsymbol{\epsilon}^{(1)}(\mathbf{x}, t)]_{pq}}{\partial x_j}, \quad (14)$$

in which  $\kappa^{(12)}(\mathbf{x}, t)$  approximates  $\mathbf{c}^{(12)}(\mathbf{x}, t)$  for small deformations.

### 2.3. Least action principle

We introduce the least action principle that will allow us to obtain the Euler-Lagrange equations. For that, we define the deformation  $\pi^{\text{def}}$ , kinetic  $\pi^{\text{kin}}$ , and external  $\pi^{\text{ext}}$  energy functionals.

It is assumed the body is submitted to Dirichlet and Neumann boundary conditions. Dirichlet conditions are applied to a part  $\partial\Omega_0$  of  $\partial\Omega$ , which implies that there are no rigid body displacements. Neumann boundary conditions are constituted of volume and surface external forces,  $\mathbf{b}^{(\Omega)}$  on  $\Omega$  and  $\mathbf{b}^{(\partial\Omega)}$  on  $\partial\Omega$ , surface external double forces,  $\mathbb{B}^{(\partial\Omega)}$  on  $\partial\Omega$ , and length external forces,  $\mathbf{b}^{(\partial\partial\Omega)}$  on  $\partial\partial\Omega$ . Note that all the Neumann boundary conditions are assumed to be zero where Dirichlet conditions are applied and that surface external double forces can be applied thanks to the use of a second-gradient model. For any fixed  $t$  in  $\mathbb{R}$ ,  $\mathbf{x} \mapsto \mathbf{u}_t(\mathbf{x}) = \mathbf{u}(\mathbf{x}, t)$  belongs to  $C_{\mathbf{u}}$ , where  $C_{\mathbf{u}}$  is the space of admissible displacements satisfying the Dirichlet condition on  $\partial\Omega_0 \subset \partial\Omega$ . Similarly, for any fixed  $t$  in  $\mathbb{R}$ ,  $\mathbf{x} \mapsto \delta\mathbf{u}_t(\mathbf{x}) = \delta\mathbf{u}(\mathbf{x}, t)$  belongs to  $C_{\delta\mathbf{u}}$ , where  $C_{\delta\mathbf{u}}$  is the space of test functions for which the Dirichlet conditions on  $\partial\Omega_0$  are equal to zero. We assume that for any fixed  $\mathbf{x}$  in  $\Omega$ ,  $t \mapsto \delta\mathbf{u}_{\mathbf{x}}(t)$  has the same regularity properties as  $t \mapsto \mathbf{u}_{\mathbf{x}}(t)$ . In the following, we

introduce initial time  $t_0$  and final time  $t_1$  for applying the least action principle, and we will assume that, for all  $\mathbf{x}$ , we have  $\delta\mathbf{u}(\mathbf{x}, t_0) = 0$  and  $\delta\mathbf{u}(\mathbf{x}, t_1) = 0$ .

**Definition 3 (Deformation energy functional).** For small deformations, assuming that the second-order derivatives are small compared to the first-order derivatives of displacement (when multiplied for the same constitutive parameter), the deformation energy functional  $\mathbf{u} \mapsto \pi^{\text{def}}(\mathbf{u})$  can be written as

$$\pi^{\text{def}}(\mathbf{u}) = \int_{t_0}^{t_1} \int_{\Omega} \phi(\mathbf{u}, \mathbf{x}, t) d\mathbf{x} dt, \quad (15)$$

where  $\phi(\mathbf{u}, \mathbf{x}, t) = \varphi(\mathbf{x}, t)$  and  $\varphi(\mathbf{x}, t)$  is defined by

$$\varphi(\mathbf{x}, t) = \frac{1}{2} \mathfrak{m}^{(0)}(\mathbf{x}) \mathfrak{a}_{ijkh}^{(11)}(\mathbf{x}) [\boldsymbol{\epsilon}^{(1)}(\mathbf{x}, t)]_{kh} [\boldsymbol{\epsilon}^{(1)}(\mathbf{x}, t)]_{ij} + \frac{1}{2} [\mathfrak{m}^{(2)}(\mathbf{x})]_{pq} \mathfrak{a}_{ijkh}^{(1212)}(\mathbf{x}) \frac{\partial [\boldsymbol{\epsilon}^{(1)}(\mathbf{x}, t)]_{kh}}{\partial x_p} \frac{\partial [\boldsymbol{\epsilon}^{(1)}(\mathbf{x}, t)]_{ij}}{\partial x_q}. \quad (16)$$

In Eq. (16),  $\mathfrak{a}^{(11)}(\mathbf{x})$  and  $\mathfrak{a}^{(1212)}(\mathbf{x})$  are fourth-order constitutive tensors defined in  $\mathbb{T}_4^+$ , and the functions  $\mathbf{x} \mapsto \mathfrak{m}^{(0)}(\mathbf{x})$  and  $\mathbf{x} \mapsto [\mathfrak{m}^{(2)}(\mathbf{x})]$  are defined by,

$$\mathfrak{m}^{(0)}(\mathbf{x}) = \int_{\Omega} \alpha(\bar{\mathbf{x}}, \mathbf{x}) d\bar{\mathbf{x}} \quad , \quad [\mathfrak{m}^{(2)}(\mathbf{x})]_{pq} = \int_{\Omega} \alpha(\bar{\mathbf{x}}, \mathbf{x}) (\bar{x}_p - x_p)(\bar{x}_q - x_q) d\bar{\mathbf{x}}. \quad (17)$$

Here, the function  $\alpha$  represents the *influence function* (also referred to as the *attenuation function*), which is chosen as

$$\alpha(\bar{\mathbf{x}}, \mathbf{x}) = \frac{1}{\xi^3 (2\pi)^{3/2}} \exp\left(-\frac{1}{2} \frac{\|\bar{\mathbf{x}} - \mathbf{x}\|^2}{\xi^2}\right), \quad (18)$$

where  $\xi$  is defined as an *interaction length*.

**Definition 4 (Kinetic energy functional).** The kinetic energy functional  $\mathbf{u} \mapsto \pi^{\text{kin}}(\mathbf{u})$  can be written as

$$\pi^{\text{kin}}(\mathbf{u}) = \int_{t_0}^{t_1} \int_{\Omega} \frac{1}{2} \rho(\mathbf{x}) \frac{\partial u_k(\mathbf{x}, t)}{\partial t} \frac{\partial u_k(\mathbf{x}, t)}{\partial t} d\mathbf{x} dt, \quad (19)$$

where  $\rho(\mathbf{x})$  denotes the mass density at  $\mathbf{x}$ .

**Definition 5 (External energy functional).** Let us call  $\mathbf{u} \mapsto \pi^{\text{ext}}(\mathbf{u})$  the external energy functional whose first variation is defined by,

$$\begin{aligned} \delta\pi^{\text{ext}}(\mathbf{u}; \delta\mathbf{u}) &= \int_{t_0}^{t_1} \int_{\Omega} b_i^{(\Omega)}(\mathbf{u}, \mathbf{x}, t) \delta u_i(\mathbf{x}, t) d\mathbf{x} dt + \int_{t_0}^{t_1} \int_{\partial\Omega} b_i^{(\partial\Omega)}(\mathbf{u}, \mathbf{x}, t) \delta u_i(\mathbf{x}, t) ds dt \\ &+ \int_{t_0}^{t_1} \int_{\partial\Omega} \mathbb{B}_i^{(\partial\Omega)}(\mathbf{u}, \mathbf{x}, t) \frac{\partial \delta u_i(\mathbf{x}, t)}{\partial \mathbf{n}} ds dt + \int_{t_0}^{t_1} \int_{\partial\partial\Omega} b_i^{(\partial\partial\Omega)}(\mathbf{u}, \mathbf{x}, t) \delta u_i(\mathbf{x}, t) d\ell dt, \end{aligned} \quad (20)$$

where, as explained before,  $\mathbf{b}^{(\Omega)}$  and  $\mathbf{b}^{(\partial\Omega)}$  are volume and surface external forces,  $\mathbb{B}^{(\partial\Omega)}$  denotes surface external double forces, and  $\mathbf{b}^{(\partial\partial\Omega)}$  stands for length external forces.

**Proposition 1 (Least action principle).** *By the least action principle, the movement is described by the displacement field  $\mathbf{u} \in C_u$  such that*

$$\delta\pi^{\text{kin}}(\mathbf{u}; \delta\mathbf{u}) - \delta\pi^{\text{def}}(\mathbf{u}; \delta\mathbf{u}) + \delta\pi^{\text{ext}}(\mathbf{u}; \delta\mathbf{u}) = 0 \quad , \quad \forall \delta\mathbf{u} \in C_{\delta\mathbf{u}}. \quad (21)$$

where  $\delta\pi^{\text{kin}}(\mathbf{u}; \delta\mathbf{u})$ ,  $\delta\pi^{\text{def}}(\mathbf{u}; \delta\mathbf{u})$ , and  $\delta\pi^{\text{ext}}(\mathbf{u}; \delta\mathbf{u})$  are the first variations of  $\pi^{\text{kin}}$ ,  $\pi^{\text{def}}$ , and  $\pi^{\text{ext}}$ , respectively.

#### 2.4. Euler-Lagrange Equations

Under the hypotheses introduced in Sections 2.2 and 2.3, the proposed theory provides a center-symmetric second-gradient model based on a two-particle interaction. Consequently, the least action principle allows us to define the effective stress tensor  $\boldsymbol{\sigma}^{\text{eff}}(\mathbf{u}, \mathbf{x}, t)$  as a function of the stress  $\boldsymbol{\sigma}(\mathbf{u}, \mathbf{x}, t)$  and the hyper stress  $\mathbb{h}(\mathbf{u}, \mathbf{x}, t)$  tensors.

**Definition 6 (Stress tensors).** Let  $\boldsymbol{\sigma}^{\text{eff}}(\mathbf{u}, \mathbf{x}, t)$  be the *effective stress tensor* represented by the matrix  $[\boldsymbol{\sigma}^{\text{eff}}(\mathbf{u}, \mathbf{x}, t)]$  in  $\mathbb{M}_3^S$  defined by

$$[\boldsymbol{\sigma}^{\text{eff}}(\mathbf{u}, \mathbf{x}, t)]_{ij} = [\boldsymbol{\sigma}(\mathbf{u}, \mathbf{x}, t)]_{ij} - \frac{\partial \mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t)}{\partial x_q}, \quad (22)$$

where  $\boldsymbol{\sigma}(\mathbf{u}, \mathbf{x}, t)$  is the *stress tensor* represented by the matrix  $[\boldsymbol{\sigma}(\mathbf{u}, \mathbf{x}, t)]$  in  $\mathbb{M}_3^S$  defined by

$$[\boldsymbol{\sigma}(\mathbf{u}, \mathbf{x}, t)]_{ij} = \mathfrak{m}^{(0)}(\mathbf{x}) \mathfrak{a}_{ijhk}^{(11)}(\mathbf{x}) \frac{\partial u_k(\mathbf{x}, t)}{\partial x_h}, \quad (23)$$

and where  $\mathfrak{h}(\mathbf{u}, \mathbf{x}, t)$  is the *hyper stress tensor* whose components are

$$\mathfrak{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) = [\mathfrak{m}^{(2)}(\mathbf{x})]_{pq} \mathfrak{a}_{ijhk}^{(1212)}(\mathbf{x}) \frac{\partial u_k(\mathbf{x}, t)}{\partial x_h \partial x_p}. \quad (24)$$

**Proposition 2 (Euler-Lagrange equations).** *The least action principle (see Proposition 1) leads to the following Euler-Lagrange equations,*

◦ on the volume  $\Omega$ ,

$$-\rho(\mathbf{x}) \frac{\partial^2 u_i(\mathbf{x}, t)}{\partial t^2} + \frac{\partial [\boldsymbol{\sigma}^{\text{eff}}(\mathbf{u}, \mathbf{x}, t)]_{ij}}{\partial x_j} + b_i^{(\Omega)}(\mathbf{u}, \mathbf{x}, t) = 0; \quad (25)$$

◦ on the boundary  $\partial\Omega$ ,

$$-[\boldsymbol{\sigma}^{\text{eff}}(\mathbf{u}, \mathbf{x}, t)]_{ij} n_j(\mathbf{x}) + \frac{\partial}{\partial x_r} \left( \mathfrak{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) n_q(\mathbf{x}) [\mathbf{p}(\mathbf{x})]_{sj} \right) [\mathbf{p}(\mathbf{x})]_{rs} + b_i^{(\partial\Omega)}(\mathbf{u}, \mathbf{x}, t) = 0, \quad (26)$$

$$-\mathfrak{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) n_q(\mathbf{x}) n_j(\mathbf{x}) + \mathbb{B}_i^{(\partial\Omega)}(\mathbf{u}, \mathbf{x}, t) = 0, \quad (27)$$

where  $[\mathbf{p}(\mathbf{x})]$  is the projection operator on tangent space;

◦ on the edges  $\partial\partial\Omega$ ,

$$-\mathfrak{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) n_q(\mathbf{x}) \nu_j(\mathbf{x}) + b_i^{(\partial\partial\Omega)}(\mathbf{u}, \mathbf{x}, t) = 0. \quad (28)$$

PROOF. See Appendix C.

**Remark 2 (Subdomain interactions).** Within the proposed theory, subdomains of the continuum interact with each other through volume and surface forces, surface double forces, and length forces. Externally applicable loads do not reduce simply to force [55]. Moreover, the effect of second-gradient terms is modulated by interaction function  $\alpha$ . Hence, the proposed theory for particle-based materials lies between integral and gradient nonlocal theories [52, 21].

### 3. Definition of an Acoustic Tensor and Its Algebraic Properties

Within the framework of classical linear elasticity for homogeneous materials, the acoustic tensor is independent of the wave number and only depends on the direction of propagation. In the context of second-order continuum models, it would depend as shown below.

**Proposition 3 (Construction of an acoustic tensor).** *Within the context of the proposed 3D second-gradient continuum model applicable to homogeneous linear elastic particle-based materials, the acoustic tensor  $\mathfrak{s}(\kappa, \mathbf{m})$  governing bulk waves in  $\mathbb{R}^3$  is represented by the following matrix (defined as the acoustic matrix)*

$$[\mathfrak{s}(\kappa, \mathbf{m})]_{ik} = \mathfrak{a}_{ijkh}^{(11)} m_h m_j + \kappa^2 \xi^2 \mathfrak{a}_{ijkh}^{(1212)} m_h m_j. \quad (29)$$

In this equation,  $\mathbf{m} = (m_1, m_2, m_3)$  is the unit vector defining the direction of propagation,  $\kappa$  is the wave number,  $\xi$  is the interaction length defined in Eq. (18),  $\mathfrak{a}_{ijkh}^{(11)}$  is the fourth-order elasticity tensor, and  $\mathfrak{a}_{ijkh}^{(1212)}$  is the one related to second-gradient effect introduced by the deformation energy density in Eq. (16).

PROOF. Let us assume that  $\Omega$  is  $\mathbb{R}^3$  and there are no external loads. Due to the properties of homogeneity, we have  $\rho(\mathbf{x}) = \rho$ ,  $\mathfrak{a}_{ijkh}^{(11)}(\mathbf{x}) = \mathfrak{a}_{ijkh}^{(11)}$  and  $\mathfrak{a}_{ijkh}^{(1212)}(\mathbf{x}) = \mathfrak{a}_{ijkh}^{(1212)}$ . Under these hypotheses, considering Eq. (17),  $\mathfrak{m}^{(0)}(\mathbf{x}) = 1$  (See Appendix B) and  $[\mathfrak{m}^{(2)}(\mathbf{x})]_{pq} = \xi^2 [\mathbb{I}]_{pq}$  are independent function of  $\mathbf{x}$ . Eq. (25) can then be simplified as

$$-\rho \frac{\partial^2 u_i(\mathbf{x}, t)}{\partial t^2} + \mathfrak{a}_{ijkh}^{(11)} \frac{\partial u_k(\mathbf{x}, t)}{\partial x_h \partial x_j} - \xi^2 [\mathbb{I}]_{pq} \mathfrak{a}_{ijkh}^{(1212)} \frac{\partial u_k(\mathbf{x}, t)}{\partial x_h \partial x_p \partial x_q \partial x_j} = 0, \quad (30)$$

which describes the propagation of bulk waves. To derive the acoustic tensor, let us consider the progressive waves defined by  $u_k(\mathbf{x}, t) = \widehat{u}_k \exp(\mathfrak{i}(\kappa \langle \mathbf{m}, \mathbf{x} \rangle - \omega t))$ , where  $\widehat{u}_k$  is a constant in  $\mathbb{C}$ ,  $\omega$  is an *angular frequency*, and  $\mathfrak{i}$  is the imaginary unit. By replacing it into (30), yields

$$(\kappa^2 \mathfrak{a}_{ijkh}^{(11)} m_h m_j + \kappa^4 \xi^2 [\mathbb{I}]_{pq} \mathfrak{a}_{ijkh}^{(1212)} m_h m_p m_q m_j - \rho \omega^2 [\mathbb{I}]_{ik}) \widehat{u}_k = 0. \quad (31)$$

Since  $[I]_{pq}m_p m_q = 1$  and introducing  $[\mathbf{s}(\kappa, \mathbf{m})]$  as defined in Eq. (29), and defining  $\widehat{\mathbf{u}} = (\widehat{u}_1, \widehat{u}_2, \widehat{u}_3)$ , Eq. (31) can be rewritten as  $([\mathbf{s}(\kappa, \mathbf{m})] - \lambda [I])\widehat{\mathbf{u}} = \mathbf{0}$ , where  $\lambda = \rho \omega^2 / \kappa^2$ . The type of this equation allows us to define  $\mathbf{s}(\kappa, \mathbf{m})$  as an acoustic tensor (note that the terminology of acoustic tensor for  $\mathbf{s}(\kappa, \mathbf{m})$  will fully be justified with Proposition 4 that defines its algebraic properties).

**Proposition 4 (Algebraic properties of the acoustic tensor and phase velocity).** *Rewriting matrix  $[\mathbf{s}(\kappa, \mathbf{m})]$  defined by Eq. (29) as*

$$[\mathbf{s}(\kappa, \mathbf{m})]_{ik} = \mathfrak{a}_{ijkh}(\kappa) m_h m_j \quad , \quad \mathfrak{a}_{ijkh}(\kappa) = \mathfrak{a}_{ijkh}^{(11)} + \kappa^2 \xi^2 \mathfrak{a}_{ijkh}^{(1212)} \quad , \quad (32)$$

for all  $\kappa > 0$  and  $\mathbf{m}$  in  $\mathbb{R}^3$  such that  $\|\mathbf{m}\| = 1$ ,  $[\mathbf{s}(\kappa, \mathbf{m})]$  is a positive-definite symmetric matrix, and  $(\lambda, \widehat{\mathbf{u}})$  is solution of the eigenvalue problem

$$([\mathbf{s}(\kappa, \mathbf{m})] - \lambda [I])\widehat{\mathbf{u}} = \mathbf{0} \quad . \quad (33)$$

There are three positive eigenvalues  $\lambda(\kappa, \mathbf{m})$ , possibly with multiplicity larger than one, which can be rewritten as  $\lambda(\kappa, \mathbf{m}) = \rho v^2(\kappa, \mathbf{m})$ , in which  $v(\kappa, \mathbf{m}) = \omega(\kappa, \mathbf{m})/\kappa$  is the phase velocity.

PROOF. Since  $\mathfrak{a}^{(11)}$  and  $\mathfrak{a}^{(1212)}$  have been assumed to be fourth-order tensors in  $\mathbb{T}_4^+$ , then  $\mathfrak{a}$  is in  $\mathbb{T}_4^+$ . For the sake of completeness, we give the proof similar to the one given in [56]. We have  $[\mathbf{s}(\kappa, \mathbf{m})]_{ki} = \mathfrak{a}_{kjih} m_j m_h$ , which can be rewritten, permuting  $j$  and  $h$ , as  $[\mathbf{s}(\kappa, \mathbf{m})]_{ki} = \mathfrak{a}_{khi j} m_h m_j$ . Since  $\mathfrak{a}_{ijkh} = \mathfrak{a}_{khi j}$ , it follows  $[\mathbf{s}(\kappa, \mathbf{m})]_{ki} = \mathfrak{a}_{ijkh} m_j m_h = [\mathbf{s}(\kappa, \mathbf{m})]_{ik}$ . Since matrix  $[\mathbf{s}(\kappa, \mathbf{m})]$  is positive definite, for  $\kappa$  and  $\mathbf{m}$  fixed, Eq. (33) appears as an eigenvalue problem of a positive-definite matrix and, consequently, the eigenvalue  $\lambda(\kappa, \mathbf{m})$  are positive, that allows the phase velocity  $v(\kappa, \mathbf{m})$  to be defined.

#### 4. Group and Phase Velocities Based on Perturbation Theory

In this section, we perform the perturbation analysis to investigate if there exist directions  $\mathbf{m}$  for which the bulk waves would be not dispersive. To simplify the writing, the dependence in  $\mathbf{m}$  is removed when this does not cause ambiguity. The dependence in  $\varepsilon = \kappa^2$  is kept because the perturbation will be performed with respect to  $\varepsilon$  around  $\varepsilon = 0$  that corresponds to the case without second-gradient effects. We are exploring the influence of second-gradient effects on the propagation of bulk waves within the framework of a perturbation theory. Let us define the matrices  $[\mathbf{s}_0]$  and  $[\mathbf{s}_1]$  such that

$$[\mathbf{s}_0]_{ik} = \mathfrak{a}_{ijkh}^{(11)} m_h m_j \quad , \quad [\mathbf{s}_1]_{ik} = \xi^2 \mathfrak{a}_{ijkh}^{(1212)} m_h m_j \quad . \quad (34)$$

Then, the acoustic matrix  $[\mathbf{s}(\varepsilon)]$  defined by Eq. (32) can be rewritten as  $[\mathbf{s}(\varepsilon)] = [\mathbf{s}_0] + \varepsilon [\mathbf{s}_1]$ .

**Proposition 5 (Perturbation of the eigenvalue problem associated with the acoustic matrix).** *Let us consider the perturbed eigenvalue problem,  $[\mathbf{s}(\varepsilon)][\boldsymbol{\psi}(\varepsilon)] = [\boldsymbol{\psi}(\varepsilon)][\boldsymbol{\lambda}(\varepsilon)]$ , for the acoustic matrix. Let  $[\mathbf{s}_0][\boldsymbol{\psi}_0] = [\boldsymbol{\psi}_0][\boldsymbol{\lambda}_0]$  be the unperturbed eigenvalue problem corresponding to  $\varepsilon = 0$ , in which  $[\boldsymbol{\lambda}_0] = [\boldsymbol{\lambda}(0)]$  is the diagonal matrix of the three positive eigenvalues of  $[\mathbf{s}_0]$  and  $[\boldsymbol{\psi}_0] = [\boldsymbol{\psi}(0)]$  is an orthogonal matrix. At  $\mathcal{O}(\varepsilon^2)$ , the perturbed eigenvalues are such that*

$$[\boldsymbol{\lambda}(\varepsilon)] = [\boldsymbol{\lambda}_0] + \varepsilon \text{diag}\{[\Delta \mathbf{s}]\} \quad , \quad [\Delta \mathbf{s}] = [\boldsymbol{\psi}_0]^T [\mathbf{s}_1] [\boldsymbol{\psi}_0] \quad , \quad (35)$$

and the perturbed eigenvectors are such that

$$[\boldsymbol{\psi}(\varepsilon)] = [\boldsymbol{\psi}_0]([I] + \varepsilon [\mathbf{q}_1]) \quad , \quad [\mathbf{q}_1]^T = -[\mathbf{q}_1] \quad . \quad (36)$$

The diagonal entries of  $[\mathbf{q}_1]$  are then zero and, if the three eigenvalues of  $[\mathbf{s}_0]$  are simple, then, the extra diagonal entries of  $[\mathbf{q}_1]$  are given by  $[\mathbf{q}_1]_{ij} = -[\Delta \mathbf{s}]_{ij} / ([\boldsymbol{\lambda}_0]_{ii} - [\boldsymbol{\lambda}_0]_{jj})$  (without summation over repeated indices).

PROOF. Let us introduce the diagonal matrix  $[\boldsymbol{\lambda}(\varepsilon)]$  of the three positive eigenvalues of  $[\mathbf{s}(\varepsilon)]$ , and the orthogonal matrix  $[\boldsymbol{\psi}(\varepsilon)]$  of the associated eigenvectors, which satisfies the perturbed eigenvalue problem,  $[\mathbf{s}(\varepsilon)][\boldsymbol{\psi}(\varepsilon)] = [\boldsymbol{\psi}(\varepsilon)][\boldsymbol{\lambda}(\varepsilon)]$ . Let  $[\mathbf{s}_0][\boldsymbol{\psi}_0] = [\boldsymbol{\psi}_0][\boldsymbol{\lambda}_0]$  be the eigenvalue problem for  $\varepsilon = 0$ , in which  $[\boldsymbol{\lambda}_0] = [\boldsymbol{\lambda}(0)]$  is the diagonal matrix of the three positive eigenvalues of  $[\mathbf{s}_0]$  and  $[\boldsymbol{\psi}_0] = [\boldsymbol{\psi}(0)]$  is an orthogonal matrix. Introducing the change of basis  $[\boldsymbol{\psi}(\varepsilon)] = [\boldsymbol{\psi}_0][\mathbf{q}(\varepsilon)]$ , the perturbed eigenvalue problem can be rewritten as

$$([\boldsymbol{\lambda}_0] + \varepsilon [\Delta \mathbf{s}])[\mathbf{q}(\varepsilon)] = [\mathbf{q}(\varepsilon)][\boldsymbol{\lambda}(\varepsilon)] \quad , \quad [\Delta \mathbf{s}] = [\boldsymbol{\psi}_0]^T [\mathbf{s}_1] [\boldsymbol{\psi}_0] \quad . \quad (37)$$

Since  $[\boldsymbol{\psi}_0]$  and  $[\boldsymbol{\psi}(\varepsilon)]$  are orthogonal matrices, it can be deduced that  $[\mathbf{q}(\varepsilon)]$  is orthogonal. The first-order perturbation of  $[\boldsymbol{\lambda}(\varepsilon)]$  and  $[\mathbf{q}(\varepsilon)]$  results in

$$[\boldsymbol{\lambda}(\varepsilon)] = [\boldsymbol{\lambda}_0] + \varepsilon [\boldsymbol{\lambda}_1] \quad , \quad [\mathbf{q}(\varepsilon)] = [I] + \varepsilon [\mathbf{q}_1] \quad . \quad (38)$$

Since  $[\mathbf{q}(\varepsilon)]$  is an orthogonal matrix, matrix  $[\mathbf{q}_1]$  must be skew-symmetric at  $\mathcal{O}(\varepsilon^2)$ , which implies that  $[\mathbf{q}_1]_{jj} = 0$  for  $j \in \{1, 2, 3\}$ . By replacing Eq. (38) into Eq. (37), we obtain at  $\mathcal{O}(\varepsilon^2)$ , the matrix equation  $[\boldsymbol{\lambda}_0][\mathbf{q}_1] + [\Delta \mathbf{s}] = [\mathbf{q}_1][\boldsymbol{\lambda}_0] + [\boldsymbol{\lambda}_1]$ . The diagonal entries of this matrix equation are  $[\boldsymbol{\lambda}_1]_{jj} = [\Delta \mathbf{s}]_{jj}$ . For  $i \neq j$ , the extra diagonal entries



of this matrix equation satisfy  $([\lambda_0]_{ii} - [\lambda_0]_{jj})[\mathbf{q}_1]_{ij} = -[\Delta \mathbf{s}]_{ij}$  (without summation over repeated Latin indices). We have then proven the proposition.

**Remark 3 (Perturbation of the phase and group velocities).** In this remark, there is no summation over repeated Latin indices. We use the definition of the phase velocity  $v = \omega/\kappa$  and the group velocity  $v^g = d\omega/d\kappa$ . The three phase velocities  $v_j(0)$  of the unperturbed system are given by

$$v_j(0) = \sqrt{[\lambda_0]_{jj}/\rho} \quad , \quad j \in \{1, 2, 3\}. \quad (39)$$

At  $O(\varepsilon^2)$ , the three phase  $v_j(\varepsilon)$  and group  $v_j^g(\varepsilon)$  velocities are written as

$$v_j(\varepsilon) \approx v_j(0) \left( 1 + \frac{\varepsilon}{2\rho} \frac{[\Delta \mathbf{s}]_{jj}}{v_j(0)^2} \right) \quad , \quad v_j^g(\varepsilon) \approx v_j(0) \left( 1 + \frac{3\varepsilon}{2\rho} \frac{[\Delta \mathbf{s}]_{jj}}{v_j(0)^2} \right) \quad , \quad j \in \{1, 2, 3\}. \quad (40)$$

We can conclude that there is no direction in which the phase velocity is equal to the group velocity, indicating a dispersive system where the group velocity exceeds the phase velocity. Consequently, for an analysis scale where second-gradient effects are not negligible, bulk waves are always dispersive.

## 5. Identification of elasticity parameters

The following procedure is inspired by [53]. The propagation of bulk waves in the anisotropic hypothesis is governed by Eq. (33). Using the abbreviated subscripts, the components  $\mathfrak{a}_{ijkh}^{(11)}$  and  $\mathfrak{a}_{ijkh}^{(1212)}$  of elasticity tensors  $\mathfrak{a}^{(11)}$  and  $\mathfrak{a}^{(1212)}$  can be expressed by the 21 components  $[\mathfrak{a}^{(1)}]_{IJ}$  and  $[\mathfrak{a}^{(2)}]_{IJ}$  of two symmetric matrices  $[\mathfrak{a}^{(1)}]$  and  $[\mathfrak{a}^{(2)}]$  with  $I$  and  $J$  in  $\{1, 2, \dots, 6\}$ . For given values of  $\kappa$  and  $\mathbf{m}$ , let us define the function  $f$  such that

$$(\xi, [\mathfrak{a}^{(1)}], [\mathfrak{a}^{(2)}]) \mapsto f(\xi, [\mathfrak{a}^{(1)}], [\mathfrak{a}^{(2)}]; \kappa, \mathbf{m}, v(\kappa, \mathbf{m})) = \det([\mathfrak{s}(\kappa, \mathbf{m})] - \lambda(\kappa, \mathbf{m})[\mathbf{I}]), \quad (41)$$

where  $\lambda(\kappa, \mathbf{m}) = \rho v^2(\kappa, \mathbf{m})$ ,  $\kappa$  and  $v(\kappa, \mathbf{m})$  represent the wave number and phase velocity. Let  $\mathcal{M} = \{(\kappa_p, \mathbf{m}_{p'})\}$ ,  $p \in \{1, \dots, N\}$ ,  $p' \in \{1, \dots, N'\}$  be the set of the  $N \times N'$  values of  $(\kappa, \mathbf{m})$  used for the measurements. For each  $(\kappa_p, \mathbf{m}_{p'}) \in \mathcal{M}$ , let  $v_{pp'} = v(\kappa_p, \mathbf{m}_{p'})$  be the measured phase velocity. The identification of  $\xi$ ,  $[\mathfrak{a}^{(1)}]$ , and  $[\mathfrak{a}^{(2)}]$  is performed by minimizing, in the mean-square sense, function  $f$  on the set  $\mathcal{M}$ . We have the proposition for the identification.

**Proposition 6.** *Identification of the constitutive matrices  $[\mathfrak{a}^{(1)}]$  and  $[\mathfrak{a}^{(2)}]$  from the measurements  $\{\kappa_p, \mathbf{m}_{p'}, v_{pp'}\}$  is performed by minimizing the functional  $F$  defined by*

$$F(\xi, [\mathfrak{a}^{(1)}], [\mathfrak{a}^{(2)}]) = \sum_{p=1}^N \sum_{p'=1}^{N'} f(\xi, [\mathfrak{a}^{(1)}], [\mathfrak{a}^{(2)}]; \kappa_p, \mathbf{m}_{p'}, v_{pp'})^2. \quad (42)$$

Since  $[\mathfrak{a}^{(1)}]$  and  $[\mathfrak{a}^{(2)}]$  are assumed to be positive definite, 12 constraints must be imposed expressed in terms of the components of  $[\mathfrak{a}^{(s)}]$ , with  $s \in \{1, 2\}$ ,

$$h_n^{(s)} = \det([\mathfrak{a}_n^{(s)}]) > 0 \quad , \quad s \in \{1, 2\} \quad , \quad n \in \{1, 2, \dots, 6\}. \quad (43)$$

Here,  $[\mathfrak{a}_n^{(s)}]$  denotes the submatrix formed by considering the first  $n$  rows and columns of  $[\mathfrak{a}^{(s)}]$ . Additionally, it is required that  $\xi > 0$  for physical consistency.

**Remark 4.** Note that the procedure just outlined provides a practical method for identifying the constitutive parameters within the framework of the proposed theory. These constitutive parameters are associated with first-gradient effects, second-gradient effects, and interaction length in the assumption of anisotropic materials.

## 6. Conclusion

In this work, we have discussed a novel center-symmetric second-gradient continuum model for particle-based materials, incorporating pairwise particle interactions. We have made the assumptions of small deformations and neglected second-order derivatives in comparison to the first ones when multiplied by the same constitutive parameters. The discussed model can be regarded as an extension of Eringen nonlocal elasticity designed to describe large interaction lengths. Furthermore, the proposed model is adaptable for large deformations, allowing the construction of  $N$ -th gradient continua when even larger interaction lengths appear. The Euler-Lagrange equations have been derived using the least action principle, offering valuable insights into non-classical interactions within subdomains. We have shown that subdomains interact through forces per unit area, double forces per unit area, forces per unit area dependent on the curvature of the Cauchy cut, and forces per unit length. We have constructed a novel, symmetric,

and positive-definite acoustic tensor that allows us to explore bulk wave propagation. The inclusion of the second-gradient term has resulted in different group and phase velocities, indicating dispersion in bulk waves. Additionally, the properties of this acoustic tensor have enabled the extension of an identification procedure from Cauchy elasticity to the proposed model, applicable to any class of symmetry. By establishing this identification procedure, we position the model for practical applications across various fields, ranging from polymers, composite materials, and liquid crystals to broader applications. Ongoing research is dedicated to the statistical identification of constitutive parameters, ensuring the robustness and applicability of the proposed model in multiple scenarios.

## Declarations

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## Appendix A

Hereafter, we undertake algebraic computations to derive Eq. (11). Starting with Eq. (4), we have

$$\begin{aligned} [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)]_{ip}[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)]_{iq} &= [\mathbf{f}^{(1)}(\mathbf{x}, t)]_{ip}[\mathbf{f}^{(1)}(\mathbf{x}, t)]_{iq} \\ &+ \frac{1}{2} \left( \frac{\partial[\mathbf{f}^{(1)}(\mathbf{x}, t)]_{ip}}{\partial x_k} [\mathbf{f}^{(1)}(\mathbf{x}, t)]_{iq} + [\mathbf{f}^{(1)}(\mathbf{x}, t)]_{ip} \frac{\partial[\mathbf{f}^{(1)}(\mathbf{x}, t)]_{iq}}{\partial x_k} \right) (\bar{x}_k - x_k) \\ &+ \frac{1}{4} \frac{\partial[\mathbf{f}^{(1)}(\mathbf{x}, t)]_{ip}}{\partial x_k} \frac{\partial[\mathbf{f}^{(1)}(\mathbf{x}, t)]_{iq}}{\partial x_s} (\bar{x}_k - x_k)(\bar{x}_s - x_s). \end{aligned} \quad (44)$$

Considering Eqs. (5) and (6) yields

$$[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)]_{ip}[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}, t)]_{iq} = [\mathbf{c}^{(1)}(\mathbf{x}, t)]_{pq} + \frac{1}{2} \mathbf{c}_{pqk}^{(12)}(\mathbf{x}, t) (\bar{x}_k - x_k) + \frac{1}{4} \mathbf{c}_{pqks}^{(2)}(\mathbf{x}, t) (\bar{x}_k - x_k)(\bar{x}_s - x_s). \quad (45)$$

Considering tensor  $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x}, t)]$ , defined by Eq. (10), results in

$$[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x}, t)]_{pq} = \frac{1}{2} \left( [\mathbf{c}^{(1)}(\mathbf{x}, t)]_{pq} - [\mathbf{I}]_{pq} \right) + \frac{1}{4} \mathbf{c}_{pqk}^{(12)}(\mathbf{x}, t) (\bar{x}_k - x_k) + \frac{1}{8} \mathbf{c}_{pqks}^{(2)}(\mathbf{x}, t) (\bar{x}_k - x_k)(\bar{x}_s - x_s), \quad (46)$$

Finally, substituting the tensors  $[\mathbf{e}^{(1)}(\mathbf{x}, t)]$ ,  $[\mathbf{e}^{(12)}(\bar{\mathbf{x}}, \mathbf{x}, t)]$ , and  $[\mathbf{e}^{(2)}(\bar{\mathbf{x}}, \mathbf{x}, t)]$ , defined by Eqs. (7), (8), and (9), we obtain Eq. (11).

## Appendix B

In this appendix, we show that  $\mathfrak{m}^{(0)}(\mathbf{x}) = 1$  in Proposition 3. Since  $\Omega$  is  $\mathbb{R}^3$ ,  $\mathfrak{m}^{(0)}(\mathbf{x})$  is given by

$$\mathfrak{m}^{(0)}(\mathbf{x}) = \int_{\mathbb{R}^3} \alpha(\bar{\mathbf{x}}, \mathbf{x}) d\bar{\mathbf{x}}, \quad (47)$$

where  $\alpha(\bar{\mathbf{x}}, \mathbf{x})$  is defined in Eq. (18). It can be seen that  $\bar{\mathbf{x}} \mapsto \alpha(\bar{\mathbf{x}}, \mathbf{x})$  is the probability density function of a Gaussian  $\mathbb{R}^3$ -valued random variable with mean vector  $\mathbf{x}$  and covariance matrix  $\xi^2 [\mathbf{I}]$ . Consequently, we have  $\mathfrak{m}^{(0)}(\mathbf{x}) = 1$ .

## Appendix C

**PROOF.** Consider  $\pi^{\text{kin}}$  defined by Eq. (19). The first variation  $\delta\pi^{\text{kin}}$  is expressed as

$$\delta\pi^{\text{kin}}(\mathbf{u}; \delta\mathbf{u}) = \int_{t_0}^{t_1} \int_{\Omega} \rho(\mathbf{x}) \frac{\partial u_k(\mathbf{x}, t)}{\partial t} \frac{\partial \delta u_k(\mathbf{x}, t)}{\partial t} d\mathbf{x} dt. \quad (48)$$

Subsequently, integrating by parts and since, for all  $\mathbf{x}$ ,  $\delta\mathbf{u}(\mathbf{x}, t_0) = 0$  and  $\delta\mathbf{u}(\mathbf{x}, t_1) = 0$ , Eq. (48) can be transformed into

$$\delta\pi^{\text{kin}}(\mathbf{u}; \delta\mathbf{u}) = - \int_{t_0}^{t_1} \int_{\Omega} \rho(\mathbf{x}) \frac{\partial^2 u_k(\mathbf{x}, t)}{\partial t^2} \delta u_k(\mathbf{x}, t) d\mathbf{x} dt. \quad (49)$$

Considering  $\pi^{\text{def}}(\mathbf{u})$ ,  $[\boldsymbol{\sigma}(\mathbf{u}, \mathbf{x}, t)]$ , and  $\mathbb{h}(\mathbf{u}, \mathbf{x}, t)$  defined in Eqs. (15), (23), and (24), the first variation  $-\delta\pi^{\text{def}}(\mathbf{u}; \delta\mathbf{u})$  is expressed as

$$-\delta\pi^{\text{def}}(\mathbf{u}; \delta\mathbf{u}) = - \int_{t_0}^{t_1} \int_{\Omega} [\boldsymbol{\sigma}(\mathbf{u}, \mathbf{x}, t)]_{ij} \frac{\partial \delta u_i(\mathbf{x}, t)}{\partial x_j} d\mathbf{x} dt - \int_{t_0}^{t_1} \int_{\Omega} \mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) \frac{\partial \delta u_i(\mathbf{x}, t)}{\partial x_j \partial x_q} d\mathbf{x} dt. \quad (50)$$

Using an integration by parts, the first integral in the right-hand side of Eq. (50) can be written as

$$\begin{aligned} - \int_{t_0}^{t_1} \int_{\Omega} [\boldsymbol{\sigma}(\mathbf{u}, \mathbf{x}, t)]_{ij} \frac{\partial \delta u_i(\mathbf{x}, t)}{\partial x_j} d\mathbf{x} dt &= - \int_{t_0}^{t_1} \int_{\partial\Omega} [\boldsymbol{\sigma}(\mathbf{u}, \mathbf{x}, t)]_{ij} n_j(\mathbf{x}) \delta u_i(\mathbf{x}, t) d\mathbf{x} dt \\ &+ \int_{t_0}^{t_1} \int_{\Omega} \frac{\partial [\boldsymbol{\sigma}(\mathbf{u}, \mathbf{x}, t)]_{ij}}{\partial x_j} \delta u_i(\mathbf{x}, t) d\mathbf{x} dt, \end{aligned} \quad (51)$$

and the second integral in the right-hand side of Eq. (50) can be expressed as

$$\begin{aligned} - \int_{t_0}^{t_1} \int_{\Omega} \mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) \frac{\partial \delta u_i(\mathbf{x}, t)}{\partial x_j \partial x_q} d\mathbf{x} dt &= - \int_{t_0}^{t_1} \int_{\partial\Omega} \mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) \frac{\partial \delta u_i(\mathbf{x}, t)}{\partial x_j} n_q(\mathbf{x}) ds dt \\ + \int_{t_0}^{t_1} \int_{\partial\Omega} \frac{\partial}{\partial x_q} (\mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t)) n_j(\mathbf{x}) \delta u_i(\mathbf{x}, t) ds dt &- \int_{t_0}^{t_1} \int_{\Omega} \frac{\partial}{\partial x_q \partial x_j} (\mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t)) \delta u_i(\mathbf{x}, t) ds dt. \end{aligned} \quad (52)$$

Let  $[\mathbf{q}(\mathbf{x})]$  and  $[\mathbf{p}(\mathbf{x})]$  denote the orthogonal and parallel projection operators, respectively. The Kronecker delta  $[\boldsymbol{\delta}]_{rj}$  is equal to the sum of  $[\mathbf{q}(\mathbf{x})]_{rj}$  and  $[\mathbf{p}(\mathbf{x})]_{rj}$ . Given that  $[\mathbf{q}(\mathbf{x})]_{rj} = n_r n_j$  and  $[\mathbf{p}(\mathbf{x})]_{rj} = [\mathbf{p}(\mathbf{x})]_{sj} [\mathbf{p}(\mathbf{x})]_{rs}$ , the first integral in the right-hand side of Eq. (52) can be transformed into

$$\begin{aligned} - \int_{t_0}^{t_1} \int_{\partial\Omega} \mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) n_q(\mathbf{x}) \frac{\partial \delta u_i(\mathbf{x}, t)}{\partial x_j} ds dt &= - \int_{t_0}^{t_1} \int_{\partial\Omega} \mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) n_j(\mathbf{x}) n_q(\mathbf{x}) \frac{\partial \delta u_i(\mathbf{x}, t)}{\partial \mathbf{n}} ds dt \\ &- \int_{t_0}^{t_1} \int_{\partial\Omega} \mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) \frac{\partial \delta u_i(\mathbf{x}, t)}{\partial x_r} ([\mathbf{p}(\mathbf{x})]_{sj} [\mathbf{p}(\mathbf{x})]_{rs}) n_q(\mathbf{x}) ds dt \end{aligned} \quad (53)$$

The second integral in the right-hand side of Eq. (53) can be rewritten as

$$\begin{aligned} &- \int_{t_0}^{t_1} \int_{\partial\Omega} \mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) \frac{\partial \delta u_i(\mathbf{x}, t)}{\partial x_r} ([\mathbf{p}(\mathbf{x})]_{sj} [\mathbf{p}(\mathbf{x})]_{rs}) n_q(\mathbf{x}) ds dt \\ &= - \int_{t_0}^{t_1} \int_{\partial\Omega} \frac{\partial}{\partial x_r} (\mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) n_q(\mathbf{x}) [\mathbf{p}(\mathbf{x})]_{sj} \delta u_i(\mathbf{x}, t)) [\mathbf{p}(\mathbf{x})]_{rs} ds dt \\ &+ \int_{t_0}^{t_1} \int_{\partial\Omega} \frac{\partial}{\partial x_r} (\mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) n_q(\mathbf{x}) [\mathbf{p}(\mathbf{x})]_{sj}) [\mathbf{p}(\mathbf{x})]_{rs} \delta u_i(\mathbf{x}, t) ds dt \end{aligned} \quad (54)$$

Using the Gauss divergence formula for bounded surfaces and since  $[\mathbf{p}(\mathbf{x})]_{sj} \nu_s(\mathbf{x}) = \nu_j(\mathbf{x})$ , the first integral in the right-hand side of Eq. (54) becomes

$$- \int_{t_0}^{t_1} \int_{\partial\Omega} \frac{\partial}{\partial x_r} (\mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) n_q(\mathbf{x}) [\mathbf{p}(\mathbf{x})]_{sj} \delta u_i(\mathbf{x}, t)) [\mathbf{p}(\mathbf{x})]_{rs} ds dt = - \int_{t_0}^{t_1} \int_{\partial\partial\Omega} \mathbb{h}_{ijq}(\mathbf{u}, \mathbf{x}, t) n_q(\mathbf{x}) \nu_j(\mathbf{x}) \delta u_i(\mathbf{x}, t) d\ell dt. \quad (55)$$

Sequentially substituting Eq. (55) into Eq. (54), Eq. (54) into Eq. (53), Eq. (53) into Eq. (52), Eqs. (52) and Eq. (51) into Eq. (50), and finally substituting Eqs. (50), (49), and (20) into Eq. (21), we obtain the Euler-Lagrange equations as presented in Proposition (2).

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