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A Higher-Order Nonlocal Elasticity Continuum Model for Deterministic and Stochastic Particle-Based Materials

Gabriele La Valle^{*1} and Christian Soize ^{†1}

¹Université Gustave Eiffel, MSME UMR 8208, 5 bd Descartes, 77454 Marne-la-Vallée, France.

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Abstract

This paper proposes, for particle-based materials, a higher-order nonlocal elasticity continuum model that includes the Piola peridynamics and the Eringen nonlocal elasticity. When referring to particle-based materials, we denote systems that can be modeled as assemblies of material points (or particles). Note that this paper is not devoted to granular materials, then factors such as the topology of contacts, granulometry, grain sizes, shapes, and geometric structure are not considered. Additionally, when referring to Piola peridynamics, we specifically denote the particular peridynamic model developed by Piola, which differs from the commonly adopted approach to peridynamics. The proposed higher-order nonlocal elasticity continuum model offers several advantages. First, it can describe interactions between material points over longer ranges than those considered by Eringen nonlocal elasticity. Second, it exhibits similar characteristics to gradient-type theories and Piola peridynamics, enabling the consideration of more complex external and contact actions, including N -th order forces and stresses. Furthermore, the proposed deterministic model is developed to lay the foundation for a stochastic formulation applicable to uncertain particle-based materials. We want to emphasize that the aim of this paper is not to unify Eringen nonlocal elasticity with the various existing peridynamic models.

1 Introduction

Nonlinear deformations of classical (or Cauchy) continua are described by means of the Green-Lagrange tensor that gives the change in length of an *infinitesimal material segment* (also named *fiber* or *material line element*) [1, 2, 3, 4, 5]. Two different approaches [6] can be listed: *Hamilton-Piola continuum mechanics* and *equilibrium-based continuum mechanics*. On the one hand, Hamilton-Piola continuum mechanics is based on the *principle of virtual work* (also known as *principle of virtual displacements* or *principle of virtual powers*) from which the equilibrium equations are derived. In this context, the principle of virtual work is acknowledged as an efficient tool, whose importance is further emphasized in [7, 8, 9, 10, 11, 12]. The pioneering contributions of Piola are foundational to Hamilton-Piola continuum mechanics, and further details can be found in [13, 14]. On the other hand, equilibrium-based continuum mechanics relies on the definition of *stress* quantities and the application of *balance laws*, which encompass the conservation laws of mass, linear momentum, and momentum of momentum [15, 16, 17]. In this context, the principle of virtual work is obtained as the weak formulation of the boundary value problem given by the equilibrium equations.

The differences between Hamilton-Piola continuum mechanics and equilibrium-based continuum mechanics become even more evident when it comes to the development of nonlocal continuum models for particle-based materials. These materials consist of an assembly of numerous solid particles, varying in sizes and shapes, and exhibit suitable properties for various applications. Specifically, Hamilton-Piola continuum mechanics is associated with the development of *Piola-like peridynamic theories*, whereas equilibrium-based continuum mechanics is linked with *Eringen-like nonlocal elasticity theories*. In general, nonlocal continuum models describe materials where the state at a point is influenced by the state of other points of the material. On the one hand, Piola-like peridynamic theories allow for the development of nonlocal continuum models that consider pairwise particle interactions without the need for the

^{*}Corresponding Author. gabrielelavalle@gmail.com

[†]christian.soize@univ-eiffel.fr

concept of stress, making them extremely suitable for multiscale modeling, structural mechanics, biomechanics, particle-based materials, and problems involving discontinuities such as cracks and interfaces [18, 19, 20, 21, 22, 23, 24]. They provide an alternative approach to formulate continuum mechanics, with roots traced back to Piola [25]. On the other hand, Eringen-like nonlocal elasticity theories [26, 27] are based on an additional principle known as *the principle of contiguity* [28]. This principle implies that the stress at a material point is determined by integrating the stress over a neighborhood surrounding that point. These models, commonly referred to as *integral nonlocal theories* [29], are applicable to continua where interaction forces rapidly decrease with distance, following the *attenuating neighborhood hypothesis* [30]. Additionally, assuming a *smooth neighborhood*, they lead to *gradient-type nonlocal theories* [28]. Applications of the Eringen and Eringen-like nonlocal elasticity theories concern nanomaterials and microstructured materials [31, 32, 33, 34]. The body of the literature on this topic is indeed extensive [35, 36, 37, 38, 39, 40].

As explained above, there exist nonlocal elasticity theories based on integral formulations (Eringen-like models) and peridynamic theories (Piola-like models). We aim to formulate a nonlocal continuum model of order N higher than one that is suitable for particle-based materials and such that: for $N = 1$, we recover the Eringen nonlocal elasticity, for $N \geq 1$, we obtain the Piola peridynamics, which does not allow Eringen nonlocal elasticity to be retrieved as a special case. The term *Piola peridynamics* refers to the particular approach to peridynamics developed by Piola [25], which differs from the commonly adopted approaches and is closely related to bond-based peridynamics [21]. Our aim is not to encompass Eringen nonlocal elasticity and peridynamics (in a broader sense) within a more comprehensive theory. Encompassing them might be challenging, given their representation of two different scales. Instead, our aim is to introduce a novel perspective to formulate nonlocal continua for particle-based materials.

Given our focus on particle-based materials, *i.e.*, materials modeled as assemblies of material points (or particles), we exclude considerations specific to granular materials. Thus, factors such as the topology of contacts, granulometry, grain sizes, shapes, and geometric structures are not taken into account.

There are two reasons for proposing this model. First, we aim to model particle interactions over a longer range than currently considered in Eringen nonlocal elasticity. Second, the proposed model accounts for more complex external and contact actions, such as N -th forces and stresses. Importantly, we achieve the desired modeling enhancement without necessitating the introduction of additional principles and without relying on the principle of contiguity used by Eringen. We introduce a second-order tensor that quantifies the change in length of a *finite* (and not infinitesimal) *material segment* and that can describe pairwise nonlocal interactions. Moreover, the proposed deterministic model has been formulated to prepare future stochastic developments devoted to particle-based materials with uncertainties concerning the constitutive properties.

The paper is structured as follows. In Section 2, we introduce a second-order tensor to describe nonlocal pairwise interactions. We then perform its polynomial decomposition to separate terms depending on the first and higher-order derivatives of the placement (or configuration) field. Furthermore, we provide its geometric interpretation. In Section 3, we compare the deformation energy density, expressed as a function of the proposed second-order tensor, with Piola and Eringen deformation energy densities, which can be obtained as particular cases. Finally, we formulate the principle of virtual work to fully characterize the proposed higher-order nonlocal continuum model for particle-based materials.

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. In particular, any second-order tensor will be represented with the matrix of its components.

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

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

The components of a fourth-order tensor \mathbf{x} will be denoted by x_{ijkl} .

This article, devoted to a deterministic formulation, is the first of the second one that will be devoted to the stochastic formulation. Consequently, the Lagrangian coordinates are denoted by boldface

lowercase instead of boldface uppercase letters, which will be reserved for the random quantities in the second part.

$\langle \mathbf{x}, \mathbf{y} \rangle$: 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 $[\mathbf{x}]$.

\wedge : vector product in \mathbb{R}^n .

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

\mathbb{M}_3 : ensemble of 3×3 real matrices.

\mathbb{M}_3^S : subset of \mathbb{M}_3 of symmetric 3×3 real matrices.

\mathbb{M}_3^+ : subset of \mathbb{M}_3^S of positive definite symmetric 3×3 real matrices.

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

2 Lagrangian Deformation Measures for Nonlocal Continua

We focus on *nonlocal particle-based materials*, specifically particle-based materials where nonlocal interparticle interactions play a significant role. Our main objective is to characterize the deformation of these materials in terms of the mutual changes in the relative positions of material points. To achieve this goal, we introduce a second-order tensor for describing pairwise nonlocal interactions. Our methodology follows the reasoning scheme of the Piola peridynamics, encompassing the following steps (see [25]): i) defining a kinematic mathematical object capable of describing symmetric pairwise interactions between material points, ii) formulating the deformation energy density as a function of this mathematical object, and iii) finalizing the nonlocal continuum model using the principle of virtual work.

2.1 Introducing a Novel Second-Order Tensor for Describing Deformation in Nonlocal Deformable Bodies

We consider a solid continuum body that occupies an open, bounded, and convex domain Ω of \mathbb{R}^3 , with a sufficiently smooth boundary $\partial\Omega$, defining the reference (or Lagrangian) configuration. Due to some external actions, Ω is transformed into the deformed (or Eulerian) configuration Ω_t . Let $\{\boldsymbol{\xi}^1, \boldsymbol{\xi}^2, \boldsymbol{\xi}^3\}$ be the canonical basis of \mathbb{R}^3 . Both reference and deformed configuration are referred to the same external Cartesian reference system $(O, \boldsymbol{\xi}^1, \boldsymbol{\xi}^2, \boldsymbol{\xi}^3)$, defined by the orthonormal basis $\{\boldsymbol{\xi}^1, \boldsymbol{\xi}^2, \boldsymbol{\xi}^3\}$, and whose generic point is $\mathbf{x} = (x_1, x_2, x_3)$. Any point \mathbf{x} in $\bar{\Omega}$ is transformed into a point $\mathbf{r}(\mathbf{x}) = (r_1(\mathbf{x}), r_2(\mathbf{x}), r_3(\mathbf{x}))$ in $\bar{\Omega}_t = \mathbf{r}(\bar{\Omega})$, where $\mathbf{x} \mapsto \mathbf{r}(\mathbf{x})$ is usually said placement (or configuration) field. Placement field $\mathbf{x} \mapsto \mathbf{r}(\mathbf{x})$ is defined from $\bar{\Omega}$ into \mathbb{R}^3 , is assumed to be a bijection from $\bar{\Omega}$ into $\bar{\Omega}_t$, to be in $\mathcal{C}^N(\Omega, \mathbb{R}^3)$, and to be such that \mathbf{r} and its N derivatives are continuous on $\bar{\Omega}$. Consequently, any point \mathbf{x} in $\bar{\Omega}$ is transformed into a unique point $\mathbf{r}(\mathbf{x})$ in $\bar{\Omega}_t$. Let us consider two particles placed at \mathbf{x} and $\bar{\mathbf{x}}$, with \mathbf{x} and $\bar{\mathbf{x}}$ in Ω . Looking at [25], Piola recognizes

$$(\bar{\mathbf{x}}, \mathbf{x}) \mapsto \varrho^2(\bar{\mathbf{x}}, \mathbf{x}) = \|\mathbf{r}(\bar{\mathbf{x}}) - \mathbf{r}(\mathbf{x})\|^2 \quad (1)$$

as an adequate function to model pairwise nonlocal interactions. With the aim of finding other suitable algebraic operators able to account for some properties of nonlocal deformation, let us consider the function $(\bar{\mathbf{x}}, \mathbf{x}) \mapsto \rho(\bar{\mathbf{x}}, \mathbf{x})$ such that

$$\rho(\bar{\mathbf{x}}, \mathbf{x}) = \|\mathbf{r}(\bar{\mathbf{x}}) - \mathbf{r}(\mathbf{x})\|^2 - \|\bar{\mathbf{x}} - \mathbf{x}\|^2, \quad (2)$$

where $\rho(\bar{\mathbf{x}}, \mathbf{x})$ defines the elongation of the *finite material segment* $\Delta\mathbf{x} = \bar{\mathbf{x}} - \mathbf{x}$ in the initial configuration, which is transformed into the finite material segment $\Delta\mathbf{r} = \mathbf{r}(\bar{\mathbf{x}}) - \mathbf{r}(\mathbf{x})$ in the deformed configuration. Let us define the indices $\alpha_1, \dots, \alpha_n$ such that $\alpha_s \in \{1, 2, 3\}$ for $s = \{1, 2, \dots, n\}$ and $n \in \mathbb{N}$. The Taylor expansion of $\mathbf{r}(\bar{\mathbf{x}})$ centered at \mathbf{x} of order N is equal to

$$\mathbf{r}(\bar{\mathbf{x}}) - \mathbf{r}(\mathbf{x}) \approx \sum_{n=1}^N \sum_{\alpha_1=1}^3 \sum_{\alpha_2=1}^3 \dots \sum_{\alpha_n=1}^3 \frac{1}{n!} \frac{\partial^n \mathbf{r}(\mathbf{x})}{\partial x_{\alpha_1} \partial x_{\alpha_2} \dots \partial x_{\alpha_n}} (\bar{x}_{\alpha_1} - x_{\alpha_1})(\bar{x}_{\alpha_2} - x_{\alpha_2}) \dots (\bar{x}_{\alpha_n} - x_{\alpha_n}). \quad (3)$$

Since Eq. (3) is invariant for any permutation of indices, we can factor out any $(\bar{\mathbf{x}}_{\alpha_s} - \mathbf{x}_{\alpha_s})$ difference. Choosing to factor out $(\bar{\mathbf{x}}_{\alpha_1} - \mathbf{x}_{\alpha_1})$ (to obtain classical elasticity for $N = 1$), we can write

$$\mathbf{r}(\bar{\mathbf{x}}) - \mathbf{r}(\mathbf{x}) = \sum_{\alpha_1=1}^3 \left(\sum_{n=1}^N \sum_{\alpha_2=1}^3 \cdots \sum_{\alpha_n=1}^3 \frac{1}{n!} \frac{\partial^n \mathbf{r}(\mathbf{x})}{\partial x_{\alpha_1} \partial x_{\alpha_2} \cdots \partial x_{\alpha_n}} (\bar{x}_{\alpha_2} - x_{\alpha_2}) \cdots (\bar{x}_{\alpha_n} - x_{\alpha_n}) \right) (\bar{x}_{\alpha_1} - x_{\alpha_1}). \quad (4)$$

We define the second-order tensor $\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})$ represented by $[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]$ in \mathbb{M}_3 such that

$$[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]_{i\alpha_1} = \sum_{n=1}^N \sum_{\alpha_2=1}^3 \cdots \sum_{\alpha_n=1}^3 \frac{1}{n!} \frac{\partial^n r_i(\mathbf{x})}{\partial x_{\alpha_1} \partial x_{\alpha_2} \cdots \partial x_{\alpha_n}} (\bar{x}_{\alpha_2} - x_{\alpha_2}) \cdots (\bar{x}_{\alpha_n} - x_{\alpha_n}), \quad (5)$$

with $i \in \{1, 2, 3\}$, as the *nonlocal deformation gradient*. Replacing Eq. (5) into Eq. (4), it yields

$$\mathbf{r}(\bar{\mathbf{x}}) \approx \mathbf{r}(\mathbf{x}) + [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] (\bar{\mathbf{x}} - \mathbf{x}). \quad (6)$$

We assume *orientation-preserving* deformation (as in classical elasticity), *i.e.*, for all \mathbf{x} in $\bar{\Omega}$,

$$\det[\mathbf{f}(\mathbf{x}, \mathbf{x})] > 0. \quad (7)$$

In addition, since Eq. (6) is an approximation, we complete the injection property of \mathbf{r} by the following hypothesis: for all $\bar{\mathbf{x}}$ and \mathbf{x} in $\bar{\Omega}$,

$$\det[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] \neq 0, \quad (8)$$

which ensures that, within the framework of this approximation, for all $\bar{\mathbf{x}}$ and \mathbf{x} in $\bar{\Omega}$ such that $\bar{\mathbf{x}} \neq \mathbf{x}$, then $\mathbf{r}(\bar{\mathbf{x}}) \neq \mathbf{r}(\mathbf{x})$, and for $\bar{\mathbf{x}} = \mathbf{x}$, then $\mathbf{r}(\bar{\mathbf{x}}) = \mathbf{r}(\mathbf{x})$. Since $\bar{\Omega}$ is a convex subset of \mathbb{R}^3 , it is also connected. Consequently, for all $\bar{\mathbf{x}}$ and \mathbf{x} in $\bar{\Omega}$, Eqs. (7) and (8) imply

$$\det[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] > 0, \quad (9)$$

by intermediate-value theorem for real continuous functions (see Theorem 4.38 in [41] pp. 87). Note that $[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]$ is not symmetric and not objective, although completely describing the deformation. In the following, we look for some quantities that are objective (that is necessary) and also symmetric (that is the choice of the proposed theory). To this purpose, we permute $\bar{\mathbf{x}}$ and \mathbf{x} in Eq. (6), yielding

$$\mathbf{r}(\mathbf{x}) \approx \mathbf{r}(\bar{\mathbf{x}}) + [\mathbf{f}(\mathbf{x}, \bar{\mathbf{x}})] (\mathbf{x} - \bar{\mathbf{x}}). \quad (10)$$

Multiplying the two members of this equation by -1 gives

$$\mathbf{r}(\bar{\mathbf{x}}) \approx \mathbf{r}(\mathbf{x}) + [\mathbf{f}(\mathbf{x}, \bar{\mathbf{x}})] (\bar{\mathbf{x}} - \mathbf{x}). \quad (11)$$

Hence, let us define the second-order tensors $\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})$ and $\mathbf{c}(\mathbf{x}, \bar{\mathbf{x}})$ represented by $[\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})]$ and $[\mathbf{c}(\mathbf{x}, \bar{\mathbf{x}})]$ in \mathbb{M}_3^+ such that

$$[\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})] = [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]^T [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})], \quad (12)$$

$$[\mathbf{c}(\mathbf{x}, \bar{\mathbf{x}})] = \frac{1}{2} ([\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})] + [\mathbf{c}(\mathbf{x}, \bar{\mathbf{x}})]). \quad (13)$$

Note that, matrices $[\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})]$ and $[\mathbf{c}(\mathbf{x}, \bar{\mathbf{x}})]$ are positive definite due to Eq. (9). Let $\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})$ be the second-order tensor represented by $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ in \mathbb{M}_3^S such that

$$[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] = \frac{1}{2} ([\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})] - [\mathbf{I}]). \quad (14)$$

Defining the second-order tensor $\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})$ whose representative matrix $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ in \mathbb{M}_3^S is given by

$$[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] = \frac{1}{2} ([\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})] - [\mathbf{I}]), \quad (15)$$

where $[\mathbf{I}]$ is the 3×3 identity matrix, it can be seen that $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ can be rewritten as

$$[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] = \frac{1}{2} ([\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] + [\mathbf{e}(\mathbf{x}, \bar{\mathbf{x}})]). \quad (16)$$

Consequently, it is equivalent to define $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ by means of the symmetrization of $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ or to define $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ using $[\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})]$ that is the symmetrization of $[\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})]$. Tensor $\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})$ and $\mathbf{c}(\mathbf{x}, \bar{\mathbf{x}})$ would correspond to the *the right Cauchy-Green tensor*, and $\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})$ and $\mathbf{e}(\mathbf{x}, \bar{\mathbf{x}})$ to the *Green-Lagrange tensor*, in a nonlocal framework. It should be noted that tensor $\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})$ might not be introduced, but we will need it

to provide the geometrical interpretation of $\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})$. Note that $(\bar{\mathbf{x}}, \mathbf{x}) \mapsto \mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})$ and $(\bar{\mathbf{x}}, \mathbf{x}) \mapsto \mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})$ are symmetric tensor fields on $\bar{\Omega} \times \bar{\Omega}$, with values in ensemble \mathbb{M}_3^+ and \mathbb{M}_3^S , respectively. Taking into account Eq. (6), yields

$$\rho(\bar{\mathbf{x}}, \mathbf{x}) \approx \langle ([\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]^T [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] - [\mathbf{I}])(\bar{\mathbf{x}} - \mathbf{x}), (\bar{\mathbf{x}} - \mathbf{x}) \rangle, \quad (17)$$

which can be rewritten, using Eq. (11), as

$$\rho(\bar{\mathbf{x}}, \mathbf{x}) \approx \langle ([\mathbf{f}(\mathbf{x}, \bar{\mathbf{x}})]^T [\mathbf{f}(\mathbf{x}, \bar{\mathbf{x}})] - [\mathbf{I}])(\bar{\mathbf{x}} - \mathbf{x}), (\bar{\mathbf{x}} - \mathbf{x}) \rangle, \quad (18)$$

Summing each member of Eqs. (17) and (18), and taking into account Eq. (13), we get

$$2\rho(\bar{\mathbf{x}}, \mathbf{x}) = \langle ([\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]^T [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] + [\mathbf{f}(\mathbf{x}, \bar{\mathbf{x}})]^T [\mathbf{f}(\mathbf{x}, \bar{\mathbf{x}})] - 2[\mathbf{I}])(\bar{\mathbf{x}} - \mathbf{x}), (\bar{\mathbf{x}} - \mathbf{x}) \rangle \quad (19)$$

and

$$\rho(\bar{\mathbf{x}}, \mathbf{x}) \approx \langle ([\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})] - [\mathbf{I}])(\bar{\mathbf{x}} - \mathbf{x}), (\bar{\mathbf{x}} - \mathbf{x}) \rangle. \quad (20)$$

Hence, taking into account Eq. (15), we are led to

$$\rho(\bar{\mathbf{x}}, \mathbf{x}) \approx \langle 2[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})](\bar{\mathbf{x}} - \mathbf{x}), (\bar{\mathbf{x}} - \mathbf{x}) \rangle. \quad (21)$$

The above equations show that the property of objectivity is satisfied. Note that symbol “ \approx ” is required since we are truncating at the order N the Taylor expansion of \mathbf{r} (see Eq. (3)). This representation allows for demonstrating that different formulated theories (Piola, Cauchy, Eringen) can be viewed through the proposed development. Specifically, it allows us to recognize $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ as a suitable mathematical object to describe pairwise interactions between material points at \mathbf{x} and $\bar{\mathbf{x}}$ and, in general, the deformation of nonlocal particle-based materials. It also contains all the information regarding the deformations that result in the elongation and shortening of finite material segment $\Delta \mathbf{x}$.

2.2 Polynomial approximation

As seen in Section 2.1, $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ depends on the N -th order derivatives of \mathbf{r} at points $\bar{\mathbf{x}}$ and \mathbf{x} . To facilitate the subsequent comparison with the Eringen nonlocal model, we now separate the terms depending on the first-order derivatives of \mathbf{r} at point \mathbf{x} from those depending on its higher-order derivatives. To achieve this, we construct a polynomial approximation of $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$. From Eq. (5), entries $[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]_{i\alpha_1}$ can be rewritten as

$$[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]_{i\alpha_1} = \frac{\partial r_i(\mathbf{x})}{\partial x_{\alpha_1}} + \sum_{n=2}^N \sum_{\alpha_2=1}^3 \cdots \sum_{\alpha_n=1}^3 \frac{1}{n!} \frac{\partial^n r_i(\mathbf{x})}{\partial x_{\alpha_1} \partial x_{\alpha_2} \cdots \partial x_{\alpha_n}} (\bar{x}_{\alpha_2} - x_{\alpha_2}) \cdots (\bar{x}_{\alpha_n} - x_{\alpha_n}), \quad (22)$$

which, defining $[\nabla \mathbf{r}(\mathbf{x})]$ in \mathbb{M}_3 such that $[\nabla \mathbf{r}(\mathbf{x})]_{i\alpha_1} = \partial r_i(\mathbf{x}) / \partial x_{\alpha_1}$, gives

$$[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]_{i\alpha_1} = [\nabla \mathbf{r}(\mathbf{x})]_{i\alpha_1} + \sum_{n=2}^N \sum_{\alpha_2=1}^3 \cdots \sum_{\alpha_n=1}^3 \frac{1}{n!} \frac{\partial^n r_i(\mathbf{x})}{\partial x_{\alpha_1} \partial x_{\alpha_2} \cdots \partial x_{\alpha_n}} (\bar{x}_{\alpha_2} - x_{\alpha_2}) \cdots (\bar{x}_{\alpha_n} - x_{\alpha_n}). \quad (23)$$

Let us define $[\Delta \mathbf{f}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]$ in \mathbb{M}_3 such that

$$[\Delta \mathbf{f}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]_{i\alpha_1} = \sum_{n=2}^N \sum_{\alpha_2=1}^3 \cdots \sum_{\alpha_n=1}^3 \frac{1}{n!} \frac{\partial^n r_i(\mathbf{x})}{\partial x_{\alpha_1} \partial x_{\alpha_2} \cdots \partial x_{\alpha_n}} (\bar{x}_{\alpha_2} - x_{\alpha_2}) \cdots (\bar{x}_{\alpha_n} - x_{\alpha_n}) \quad (24)$$

to group terms depending on derivatives of \mathbf{r} at point \mathbf{x} of second-order and higher-order. Replacing Eq. (24) into Eq. (23), we get

$$[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] = [\nabla \mathbf{r}(\mathbf{x})] + [\Delta \mathbf{f}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]. \quad (25)$$

Now, let us derive Eq. (6) with respect to $\bar{\mathbf{x}}$ to obtain

$$\frac{\partial r_i(\bar{\mathbf{x}})}{\partial \bar{x}_j} = \sum_{\alpha_1=1}^3 \frac{\partial [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]_{i\alpha_1}}{\partial \bar{x}_j} (\bar{x}_{\alpha_1} - x_{\alpha_1}) + [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]_{ij}, \quad (26)$$

with i and j in $\{1, 2, 3\}$, and let us consider Eq. (25) to get

$$\frac{\partial r_i(\bar{\mathbf{x}})}{\partial \bar{x}_j} = \sum_{\alpha_1=1}^3 \frac{\partial [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]_{i\alpha_1}}{\partial \bar{x}_j} (\bar{x}_{\alpha_1} - x_{\alpha_1}) + \frac{\partial r_i(\mathbf{x})}{\partial x_j} + [\Delta \mathbf{f}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]_{ij}. \quad (27)$$

Defining $[\Delta \mathbf{h}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]$ in \mathbb{M}_3 such that

$$[\Delta \mathbf{h}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]_{ij} = \sum_{\alpha_1=1}^3 \frac{\partial [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]_{i\alpha_1}}{\partial \bar{x}_j} (\bar{x}_{\alpha_1} - x_{\alpha_1}) + [\Delta \mathbf{f}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]_{ij}, \quad (28)$$

yields

$$[\nabla \mathbf{r}(\bar{\mathbf{x}})] = [\nabla \mathbf{r}(\mathbf{x})] + [\Delta \mathbf{h}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})], \quad (29)$$

where $[\nabla \mathbf{r}(\bar{\mathbf{x}})]_{i\alpha_1} = \partial r_i(\bar{\mathbf{x}}) / \partial \bar{x}_{\alpha_1}$. Taking into account Eqs. (12) and (25), Eq. (13) becomes

$$\begin{aligned} [\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})] &= \frac{1}{2}([\nabla \mathbf{r}(\mathbf{x})]^T + [\Delta \mathbf{f}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]^T)([\nabla \mathbf{r}(\mathbf{x})] + [\Delta \mathbf{f}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]) \\ &+ \frac{1}{2}([\nabla \mathbf{r}(\bar{\mathbf{x}})]^T + [\Delta \mathbf{f}(\bar{\mathbf{x}}, \mathbf{x} - \bar{\mathbf{x}})]^T)([\nabla \mathbf{r}(\bar{\mathbf{x}})] + [\Delta \mathbf{f}(\bar{\mathbf{x}}, \mathbf{x} - \bar{\mathbf{x}})]). \end{aligned} \quad (30)$$

Hence, considering Eq. (29), Eq. (30) can be rewritten as

$$\begin{aligned} [\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})] &= \frac{1}{2}([\nabla \mathbf{r}(\mathbf{x})]^T + [\Delta \mathbf{f}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]^T)([\nabla \mathbf{r}(\mathbf{x})] + [\Delta \mathbf{f}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]) \\ &+ \frac{1}{2}([\nabla \mathbf{r}(\mathbf{x})]^T + [\Delta \mathbf{h}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})]^T + [\Delta \mathbf{f}(\bar{\mathbf{x}}, \mathbf{x} - \bar{\mathbf{x}})]^T)([\nabla \mathbf{r}(\mathbf{x})] + [\Delta \mathbf{h}(\mathbf{x}, \bar{\mathbf{x}} - \mathbf{x})] + [\Delta \mathbf{f}(\bar{\mathbf{x}}, \mathbf{x} - \bar{\mathbf{x}})]). \end{aligned} \quad (31)$$

Let $[\mathbf{c}^{(1)}(\mathbf{x})]$ in \mathbb{M}_3^+ be the matrix representing the *right Cauchy-Green tensor* $\mathbf{c}^{(1)}(\mathbf{x})$, defined by

$$[\mathbf{c}^{(1)}(\mathbf{x})] = [\nabla \mathbf{r}(\mathbf{x})]^T [\nabla \mathbf{r}(\mathbf{x})], \quad (32)$$

and let $[\Delta \mathbf{c}(\mathbf{x}, \bar{\mathbf{x}}, \bar{\mathbf{x}} - \mathbf{x})]$ in \mathbb{M}_3^S defined by

$$[\Delta \mathbf{c}(\mathbf{x}, \bar{\mathbf{x}}, \bar{\mathbf{x}} - \mathbf{x})] = [\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})] - [\mathbf{c}^{(1)}(\mathbf{x})], \quad (33)$$

in which $[\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})]$ is given by Eq. (31), which depends on \mathbf{x} , $\bar{\mathbf{x}}$, and $\bar{\mathbf{x}} - \mathbf{x}$. Finally, let us introduce $[\mathbf{e}^{(1)}(\mathbf{x})]$ in \mathbb{M}_3^S representing the *Lagrangian-Green tensor* $\mathbf{e}^{(1)}(\mathbf{x})$, defined by

$$[\mathbf{e}^{(1)}(\mathbf{x})] = \frac{1}{2}([\mathbf{c}^{(1)}(\mathbf{x})] - [\mathbf{I}]), \quad (34)$$

and $[\Delta \mathbf{e}(\mathbf{x}, \bar{\mathbf{x}}, \bar{\mathbf{x}} - \mathbf{x})]$ in \mathbb{M}_3^S such that

$$[\Delta \mathbf{e}(\mathbf{x}, \bar{\mathbf{x}}, \bar{\mathbf{x}} - \mathbf{x})] = [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] - [\mathbf{e}^{(1)}(\mathbf{x})]. \quad (35)$$

It can be deduced that

$$[\Delta \mathbf{e}(\mathbf{x}, \bar{\mathbf{x}}, \bar{\mathbf{x}} - \mathbf{x})] = \frac{1}{2}[\Delta \mathbf{c}(\mathbf{x}, \bar{\mathbf{x}}, \bar{\mathbf{x}} - \mathbf{x})]. \quad (36)$$

Note that $[\mathbf{c}(\mathbf{x}, \mathbf{x})] = [\mathbf{c}^{(1)}(\mathbf{x})]$, and consequently $[\Delta \mathbf{e}(\mathbf{x}, \mathbf{x}, \mathbf{0})] = \mathbf{0}$. Using the properties introduced for \mathbf{r} and since $\bar{\Omega}$ is a compact set in \mathbb{R}^3 , it can easily be proven that, for all i, j , and for all \mathbf{x} in Ω ,

$$\lim_{\bar{\mathbf{x}} \rightarrow \mathbf{x}} \frac{|[\Delta \mathbf{e}(\mathbf{x}, \bar{\mathbf{x}}, \bar{\mathbf{x}} - \mathbf{x})]_{ij}|}{\|\bar{\mathbf{x}} - \mathbf{x}\|} = k_{ij}(\mathbf{x}) \leq k_0 < +\infty \quad (37)$$

in which the positive-valued function k_{ij} , which could be zero at given \mathbf{x} , is bounded by $k_0 > 0$ on $\bar{\Omega}$. Thus, $[\Delta \mathbf{e}(\mathbf{x}, \bar{\mathbf{x}}, \bar{\mathbf{x}} - \mathbf{x})]_{ij}$ is $O(\|\bar{\mathbf{x}} - \mathbf{x}\|)$ or $o(\|\bar{\mathbf{x}} - \mathbf{x}\|)$ for $\bar{\mathbf{x}} \rightarrow \mathbf{x}$. In short, we will write that $[\Delta \mathbf{e}(\mathbf{x}, \bar{\mathbf{x}}, \bar{\mathbf{x}} - \mathbf{x})]_{ij}$ is $\mathcal{O}(\|\bar{\mathbf{x}} - \mathbf{x}\|)$ for $\bar{\mathbf{x}} \rightarrow \mathbf{x}$. In the following, Eq. (37) will be used to obtain the Eringen nonlocal elasticity theory as a particular case of the proposed higher-order nonlocal continuum model for particle-based materials.

2.3 Geometrical Interpretation of $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$: Length, Angle, Volume, and Surface Changes.

Matrix $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ (see Eq. (15)) has a similar geometric interpretation as $[\mathbf{e}^{(1)}(\mathbf{x})]$ (see Eq. (34)) when considering finite (and not infinitesimal) segments. Let \mathbf{m} be a unit vector in \mathbb{R}^3 . Let us consider the finite segment $\Delta \mathbf{x}^{\mathbf{m}}$ such that $\Delta \mathbf{x}^{\mathbf{m}} = \langle \Delta \mathbf{x}, \mathbf{m} \rangle \mathbf{m}$, with $\Delta \mathbf{x} = \bar{\mathbf{x}} - \mathbf{x}$. Let us define the vector

$$\Delta \mathbf{r}^{\mathbf{m}} = [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] \Delta \mathbf{x}^{\mathbf{m}}, \quad (38)$$

which can be interpreted as the deformed configuration of $\Delta \mathbf{x}^{\mathbf{m}}$ due to the movement of $\bar{\mathbf{x}}$ with respect to \mathbf{x} described by $[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]$. Note that $\Delta \mathbf{x}^{\mathbf{m}}$ and $\Delta \mathbf{r}^{\mathbf{m}}$ are not the projections of $\Delta \mathbf{x}$ and $\Delta \mathbf{r}$ on \mathbf{m} , and will

be not *material* segments if they do not belong to $\bar{\Omega}$ and $\bar{\Omega}_t$, respectively. Let $\ell^{\mathbf{m}}$ be the finite relative elongation defined by

$$\ell^{\mathbf{m}} = \frac{\|\Delta \mathbf{r}^{\mathbf{m}}\| - \|\Delta \mathbf{x}^{\mathbf{m}}\|}{\|\Delta \mathbf{x}^{\mathbf{m}}\|}, \quad (39)$$

which depends on $\bar{\mathbf{x}}$ and \mathbf{x} . Taking into account Eqs. (12) and (14), we get

$$\frac{\|\Delta \mathbf{r}^{\mathbf{m}}\|^2 - \|\Delta \mathbf{x}^{\mathbf{m}}\|^2}{\|\Delta \mathbf{x}^{\mathbf{m}}\|^2} = \langle 2[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] \mathbf{m}, \mathbf{m} \rangle, \quad (40)$$

where $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ is defined in Eq. (14), and Eq. (40) can be rewritten as,

$$\ell^{\mathbf{m}}(\ell^{\mathbf{m}} + 2) - \langle 2[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] \mathbf{m}, \mathbf{m} \rangle = 0. \quad (41)$$

Using Eqs. (14), (12), and (9) yield $1 + \langle 2[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] \mathbf{m}, \mathbf{m} \rangle = \langle [\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})] \mathbf{m}, \mathbf{m} \rangle = \|[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] \mathbf{m}\|^2 > 0$. Consequently, the two solutions of Eq. (41) are real. Choosing the physically admissible solution of this equation (eliminating the solution that is always negative), yields

$$\ell^{\mathbf{m}} = -1 + \sqrt{1 + \langle 2[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] \mathbf{m}, \mathbf{m} \rangle}. \quad (42)$$

Consequently, if \mathbf{m} is chosen as $\boldsymbol{\xi}^i$, with $i \in \{1, 2, 3\}$, we get

$$\ell^{\boldsymbol{\xi}^i} = -1 + \sqrt{1 + 2[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{ii}}. \quad (43)$$

Now, let $\tilde{\mathbf{m}}$ be another unit vector. Let us consider the finite segment $\Delta \mathbf{x}^{\tilde{\mathbf{m}}}$ such that $\Delta \mathbf{x}^{\tilde{\mathbf{m}}} = |\langle \Delta \mathbf{x}, \tilde{\mathbf{m}} \rangle| \tilde{\mathbf{m}}$ and the vector $\Delta \mathbf{r}^{\tilde{\mathbf{m}}} = [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] \Delta \mathbf{x}^{\tilde{\mathbf{m}}}$. Moreover, let us define $\vartheta^{\mathbf{m}\tilde{\mathbf{m}}}$ in $[0, \pi]$ such that

$$\cos \vartheta^{\mathbf{m}\tilde{\mathbf{m}}} = \left\langle \frac{\Delta \mathbf{r}^{\mathbf{m}}}{\|\Delta \mathbf{r}^{\mathbf{m}}\|}, \frac{\Delta \mathbf{r}^{\tilde{\mathbf{m}}}}{\|\Delta \mathbf{r}^{\tilde{\mathbf{m}}}\|} \right\rangle. \quad (44)$$

Taking into account Eqs. (12) and (14), Eq. (44) can be rewritten as

$$\cos \vartheta^{\mathbf{m}\tilde{\mathbf{m}}} = \frac{\langle ([I] + 2[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]) \mathbf{m}, \tilde{\mathbf{m}} \rangle}{\sqrt{1 + 2\langle [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] \mathbf{m}, \mathbf{m} \rangle} \sqrt{1 + 2\langle [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] \tilde{\mathbf{m}}, \tilde{\mathbf{m}} \rangle}}. \quad (45)$$

For $i \neq j$, if $\mathbf{m} = \boldsymbol{\xi}^i$ and $\tilde{\mathbf{m}} = \boldsymbol{\xi}^j$, then

$$\cos \vartheta^{\boldsymbol{\xi}^i \boldsymbol{\xi}^j} = \frac{2[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{ij}}{\sqrt{1 + 2[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{ii}} \sqrt{1 + 2[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{jj}}}. \quad (46)$$

We conclude that the entries of $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ can describe the discrepancy between the finite parallelepiped \mathbf{p} defined by the three segments $\Delta \mathbf{x}^{\boldsymbol{\xi}^i} = |\langle \Delta \mathbf{x}, \boldsymbol{\xi}^i \rangle| \boldsymbol{\xi}^i = |\Delta x_i| \boldsymbol{\xi}^i$, with $i \in \{1, 2, 3\}$, and the finite parallelepiped \mathbf{p}_t defined by the three segments $\Delta \mathbf{r}^{\boldsymbol{\xi}^i} = [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] \Delta \mathbf{x}^{\boldsymbol{\xi}^i}$, with $i \in \{1, 2, 3\}$. This discrepancy is caused by the deformation resulting from the displacements of $\bar{\mathbf{x}}$ with respect to \mathbf{x} , which is described by $[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]$. Consequently, in a more accurate way, $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ describes the discrepancy between \mathbf{p} and \mathbf{p}_t caused by the deformation resulting not only from the displacements of $\bar{\mathbf{x}}$ with respect to \mathbf{x} , but also of \mathbf{x} with respect to $\bar{\mathbf{x}}$, which is described by both $[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]$ and $[\mathbf{f}(\mathbf{x}, \bar{\mathbf{x}})]$.

Eq. (9) implies that $\{\Delta \mathbf{r}^{\boldsymbol{\xi}^1}, \Delta \mathbf{r}^{\boldsymbol{\xi}^2}, \Delta \mathbf{r}^{\boldsymbol{\xi}^3}\}$ preserves the same orientation of the right-handed triplet of finite segments $\{\Delta \mathbf{x}^{\boldsymbol{\xi}^1}, \Delta \mathbf{x}^{\boldsymbol{\xi}^2}, \Delta \mathbf{x}^{\boldsymbol{\xi}^3}\}$. The change in volume between \mathbf{p} and \mathbf{p}_t is described by $\det([\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})])$. Moreover, Eq. (9) implies that the polar decomposition of $[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]$ results in $[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] = [\mathbf{q}(\bar{\mathbf{x}}, \mathbf{x})][\mathbf{v}(\bar{\mathbf{x}}, \mathbf{x})]$, where $[\mathbf{v}(\bar{\mathbf{x}}, \mathbf{x})] = [\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})]^{1/2}$ (see Eq. (12)) and $[\mathbf{q}(\bar{\mathbf{x}}, \mathbf{x})]$ is a special orthogonal matrix that describes the rigid rotation in the configuration change from \mathbf{p} to \mathbf{p}_t induced by $[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]$.

Now, let us consider the planar surface element defined by $\Delta \mathbf{x}^{\boldsymbol{\xi}^1}$ and $\Delta \mathbf{x}^{\boldsymbol{\xi}^2}$. Let $\Delta s^{\boldsymbol{\xi}^1 \boldsymbol{\xi}^2}$ be its area and, thus, $\boldsymbol{\xi}^3$ is the unit normal to this plane. Similarly, if $\Delta s_t^{\boldsymbol{\xi}^1 \boldsymbol{\xi}^2}$ and $\boldsymbol{\xi}_t^3$ are the area and the unit normal, respectively, to the planar surface defined by $\Delta \mathbf{r}^{\boldsymbol{\xi}^1} = [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] \Delta \mathbf{x}^{\boldsymbol{\xi}^1}$ and $\Delta \mathbf{r}^{\boldsymbol{\xi}^2} = [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})] \Delta \mathbf{x}^{\boldsymbol{\xi}^2}$, then, usual algebraic calculations show that

$$\Delta s_t^{\boldsymbol{\xi}^1 \boldsymbol{\xi}^2} \boldsymbol{\xi}_t^3 = \Delta s^{\boldsymbol{\xi}^1 \boldsymbol{\xi}^2} \det([\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]) [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]^{-T} \boldsymbol{\xi}^3. \quad (47)$$

Eq. (47) would correspond to the *Piola formula* (this formula is commonly attributed to Nanson in the literature, a misattribution discussed in [42]) in a nonlocal framework.

3 Nonlocal Deformation Energies and The Principle of Virtual Work

Acknowledging the importance of the principle of virtual work, our focus lies in constructing a deformation energy density within the framework of the proposed theory.

First, we introduce the deformation energy density implied by the Eringen and Piola nonlocal models. Second, we present a deformation energy density that could encompass both the Piola and Eringen deformation energy densities as particular cases. Finally, we formulate the principle of virtual work, providing a comprehensive characterization of the proposed higher-order nonlocal continuum model for particle-based materials.

3.1 Eringen Nonlocal Elasticity Deformation Energy Density

The deformation energy density $w([\boldsymbol{\varepsilon}(\bar{\mathbf{x}})], [\boldsymbol{\varepsilon}(\mathbf{x})], \bar{\mathbf{x}}, \mathbf{x})$ pertaining a body of nonlocal, linear, elastic, macroscopic homogeneous particle-based material is expressed by Eringen as (see [30], pp. 80, and [35])

$$w([\boldsymbol{\varepsilon}(\bar{\mathbf{x}})], [\boldsymbol{\varepsilon}(\mathbf{x})], \bar{\mathbf{x}}, \mathbf{x}) = \frac{1}{2} \sum_{i,j,k,h=1}^3 \alpha(\|\bar{\mathbf{x}} - \mathbf{x}\|) \lambda_{ijkl} [\boldsymbol{\varepsilon}(\bar{\mathbf{x}})]_{kh} [\boldsymbol{\varepsilon}(\mathbf{x})]_{ij}, \quad (48)$$

where $[\boldsymbol{\varepsilon}(\mathbf{x})]$ approximates $[\mathbf{e}^{(1)}(\mathbf{x})]$ under the hypothesis of small deformations, and $\boldsymbol{\lambda}$ is the fourth-order elasticity tensor independent of $\bar{\mathbf{x}}$ and \mathbf{x} , which satisfies the usual properties of symmetry,

$$\lambda_{ijkl} = \lambda_{jikl} = \lambda_{ijlk} = \lambda_{klij}. \quad (49)$$

Function $y \mapsto \alpha(y)$ is usually named *influence function* (or *attenuation/kernel function*), is such that $\alpha(0) = 1$, and it acknowledges the phenomenon of decreasing interaction forces with the distance (see the attenuating neighborhood hypothesis in [30] pp. 34). In Eq. (48), the *macroscopic homogeneity* of materials accounts for the fact that $\alpha(\|\bar{\mathbf{x}} - \mathbf{x}\|) \lambda_{ijkl}$ depends on the couple $(\bar{\mathbf{x}}, \mathbf{x})$ only through $\|\bar{\mathbf{x}} - \mathbf{x}\|$ (rotation invariance (see [28, 39])). However, Eringen chose to keep the first-order approximation of α in Eq. (48) (see [30], pp. 76), *i.e.*, α must rapidly attenuate with distance and $\mathcal{O}(\|\bar{\mathbf{x}} - \mathbf{x}\|^2)$ are negligible.

3.2 Piola Peridynamics Deformation Energy Density

From [25], Piola defines the deformation energy density $\psi(\varrho^2(\bar{\mathbf{x}}, \mathbf{x}), \bar{\mathbf{x}}, \mathbf{x})$ as a function of $\varrho^2(\bar{\mathbf{x}}, \mathbf{x})$ (see Eq. (1)). Since $\varrho^2(\bar{\mathbf{x}}, \mathbf{x})$ is a function of $\rho(\bar{\mathbf{x}}, \mathbf{x})$ (see Eq. (2)), it exists a function $(\rho(\bar{\mathbf{x}}, \mathbf{x}), \bar{\mathbf{x}}, \mathbf{x}) \mapsto w(\rho(\bar{\mathbf{x}}, \mathbf{x}), \bar{\mathbf{x}}, \mathbf{x})$ such that $w(\rho(\bar{\mathbf{x}}, \mathbf{x}), \bar{\mathbf{x}}, \mathbf{x}) = \psi(\varrho^2(\bar{\mathbf{x}}, \mathbf{x}), \bar{\mathbf{x}}, \mathbf{x})$. Among all possible alternatives, we focus on the case for which $w(\rho(\bar{\mathbf{x}}, \mathbf{x}), \bar{\mathbf{x}}, \mathbf{x})$ is the following quadratic function in $\rho(\bar{\mathbf{x}}, \mathbf{x})$,

$$w(\rho(\bar{\mathbf{x}}, \mathbf{x}), \bar{\mathbf{x}}, \mathbf{x}) = \frac{1}{8} k(\bar{\mathbf{x}}, \mathbf{x}) \rho^2(\bar{\mathbf{x}}, \mathbf{x}). \quad (50)$$

Defining the fourth-order tensor $\mathbf{b}(\bar{\mathbf{x}}, \mathbf{x})$ such that

$$b_{ijkl}(\bar{\mathbf{x}}, \mathbf{x}) = (\bar{x}_i - x_i)(\bar{x}_j - x_j)(\bar{x}_k - x_k)(\bar{x}_l - x_l), \quad (51)$$

and taking into account Eq. (21), we get

$$w(\rho(\bar{\mathbf{x}}, \mathbf{x}), \bar{\mathbf{x}}, \mathbf{x}) = \frac{1}{2} \sum_{i,j,k,h=1}^3 k(\bar{\mathbf{x}}, \mathbf{x}) b_{ijkl}(\bar{\mathbf{x}}, \mathbf{x}) [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{kh} [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{ij}. \quad (52)$$

Although Eq. (52) does not explicitly appear in the work of Piola (see [13, 14]), we refer to it as *Piola peridynamics deformation energy density*. Note that Eqs. (52) and (48) related to deformation energy densities cannot be compared and are associated with different scales of modeling.

3.3 Proposed Nonlocal Elasticity Deformation Energy Density

We propose to directly define the deformation energy density $\varphi([\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})], \bar{\mathbf{x}}, \mathbf{x})$ as a function of $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$. Note that under this hypothesis, the deformation energy density is not explicitly a function of the position function \mathbf{r} in \mathbf{x} and $\bar{\mathbf{x}}$, as in Piola peridynamics, but is explicitly a function of the derivatives of \mathbf{r} , as in classical (or Cauchy) elasticity. It is crucial to emphasize that the novel model is developed within the

framework of continuum and not discrete mechanics. Focusing on the case for which $\varphi([\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})], \bar{\mathbf{x}}, \mathbf{x})$ is a quadratic function of $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$, yields

$$\varphi([\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})], \bar{\mathbf{x}}, \mathbf{x}) = \frac{1}{2} \sum_{i,j,k,h=1}^3 a_{ijkl}(\bar{\mathbf{x}}, \mathbf{x}) [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{kh} [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{ij}, \quad (53)$$

where $\mathbf{a}(\bar{\mathbf{x}}, \mathbf{x})$ is a fourth-order tensor that satisfies the usual properties of symmetry,

$$a_{ijkl}(\bar{\mathbf{x}}, \mathbf{x}) = a_{jikl}(\bar{\mathbf{x}}, \mathbf{x}) = a_{ijlk}(\bar{\mathbf{x}}, \mathbf{x}) = a_{klij}(\bar{\mathbf{x}}, \mathbf{x}). \quad (54)$$

In the following, we show that Piola and Eringen continuum models can be obtained from the proposed formulation (see Section 3.3.1 and Section 3.3.2). It is evident that obtaining classical (or Cauchy) elastic model as a particular case is also possible. Eq. (53) generalizes Eringen model for $N \geq 1$. Eq. (53) also generalizes Eringen model, which is formulated for $N = 1$, when influence functions do not satisfy the attenuating neighborhood hypothesis as given in Section 3.1., *i.e.*, for long-range interactions. Hence, it allows us to model all the materials in which interaction forces decrease with distance inside an interaction domain, usually named *cohesive zone* (see [30]), larger than the one allowed by Eringen model. In addition, the proposed model allows the deterministic case to be extended to the stochastic one in modeling $\mathbf{a}(\bar{\mathbf{x}}, \mathbf{x})$ by random fields using well-established techniques in [43, 44, 45, 46, 47, 48].

3.3.1 Piola Peridynamics Deformation Energy Density as a Particular Case

Let us consider Eqs. (52) and (53). If $\mathbf{a}(\bar{\mathbf{x}}, \mathbf{x}) = k(\bar{\mathbf{x}}, \mathbf{x})\mathbf{b}(\bar{\mathbf{x}}, \mathbf{x})$, Eq. (53) is reduced to the Piola peridynamics deformation energy density as given in Eq. (52),

$$\varphi([\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})], \bar{\mathbf{x}}, \mathbf{x}) = \frac{1}{2} \sum_{i,j,k,h=1}^3 k(\bar{\mathbf{x}}, \mathbf{x}) b_{ijkl}(\bar{\mathbf{x}}, \mathbf{x}) [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{kh} [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{ij}. \quad (55)$$

Note that tensor $\mathbf{b}(\bar{\mathbf{x}}, \mathbf{x})$, defined in Eq. (51), is a fourth-order tensor that not only satisfies the usual properties of symmetry,

$$b_{ijkl}(\bar{\mathbf{x}}, \mathbf{x}) = b_{jikl}(\bar{\mathbf{x}}, \mathbf{x}) = b_{ijlk}(\bar{\mathbf{x}}, \mathbf{x}) = b_{klij}(\bar{\mathbf{x}}, \mathbf{x}), \quad (56)$$

but also

$$b_{ijkl}(\bar{\mathbf{x}}, \mathbf{x}) = b_{hjkil}(\bar{\mathbf{x}}, \mathbf{x}) = b_{ikjhl}(\bar{\mathbf{x}}, \mathbf{x}). \quad (57)$$

Historically, the pioneering work of Piola laid the groundwork for peridynamics and nonlocal continuum theories [49]. This work does not aim to discuss the superiority of one theory over another, but rather to analyze the property of a novel nonlocal continuum model by comparing it to Piola peridynamics and Eringen nonlocal elasticity.

3.3.2 Eringen Nonlocal Elasticity Deformation Energy Density as a Particular Case

Let us consider Eqs. (48) and (53). Assuming $\mathbf{a}(\bar{\mathbf{x}}, \mathbf{x}) = \alpha(\|\bar{\mathbf{x}} - \mathbf{x}\|)\boldsymbol{\lambda}$ and recalling that $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] = [\mathbf{e}(\mathbf{x}, \bar{\mathbf{x}})]$, Eq. (53) becomes

$$\varphi([\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})], \bar{\mathbf{x}}, \mathbf{x}) = \frac{1}{2} \sum_{i,j,k,h=1}^3 \alpha(\|\bar{\mathbf{x}} - \mathbf{x}\|) \lambda_{ijkl} [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{kh} [\mathbf{e}(\mathbf{x}, \bar{\mathbf{x}})]_{ij}. \quad (58)$$

Let us highlight that α is an influence function rapidly decreasing with distance such that terms $\mathcal{O}(\|\bar{\mathbf{x}} - \mathbf{x}\|^2)$ can be neglected (see Section 3.1). To show that Eq. (58) can be reduced to Eq. (48) under the hypothesis of small deformations, we study two scenarios following the Eringen development by neglecting the quadratic terms $\mathcal{O}(\|\bar{\mathbf{x}} - \mathbf{x}\|^2)$: i) $\mathbf{x} \neq \bar{\mathbf{x}}$ and ii) $\mathbf{x} = \bar{\mathbf{x}}$.

i) If $\mathbf{x} \neq \bar{\mathbf{x}}$, dividing and multiplying by $\|\bar{\mathbf{x}} - \mathbf{x}\|^2$, then

$$\varphi([\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})], \bar{\mathbf{x}}, \mathbf{x}) = \frac{1}{2} \sum_{i,j,k,h=1}^3 \frac{1}{\|\bar{\mathbf{x}} - \mathbf{x}\|^2} \alpha(\|\bar{\mathbf{x}} - \mathbf{x}\|) \lambda_{ijkl} \left(\|\bar{\mathbf{x}} - \mathbf{x}\| [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{kh} \right) \left(\|\bar{\mathbf{x}} - \mathbf{x}\| [\mathbf{e}(\mathbf{x}, \bar{\mathbf{x}})]_{ij} \right). \quad (59)$$

Taking into account the polynomial decomposition of $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ (see Eq. (35)), Eq. (59) can be rewritten as

$$\begin{aligned} \varphi([\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})], \bar{\mathbf{x}}, \mathbf{x}) &= \frac{1}{2} \sum_{i,j,k,h=1}^3 \frac{1}{\|\bar{\mathbf{x}} - \mathbf{x}\|^2} \alpha(\|\bar{\mathbf{x}} - \mathbf{x}\|) \lambda_{ijkh} \left(\|\bar{\mathbf{x}} - \mathbf{x}\| [\mathbf{e}^{(1)}(\bar{\mathbf{x}})]_{kh} + \|\bar{\mathbf{x}} - \mathbf{x}\| [\Delta \mathbf{e}(\mathbf{x}, \bar{\mathbf{x}}, \bar{\mathbf{x}} - \mathbf{x})]_{kh} \right) \\ &\quad \times \left(\|\bar{\mathbf{x}} - \mathbf{x}\| [\mathbf{e}^{(1)}(\mathbf{x})]_{ij} + \|\bar{\mathbf{x}} - \mathbf{x}\| [\Delta \mathbf{e}(\bar{\mathbf{x}}, \mathbf{x}, \mathbf{x} - \bar{\mathbf{x}})]_{ij} \right). \end{aligned} \quad (60)$$

Thanks to property (37), Eq. (59) becomes

$$\begin{aligned} \varphi([\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})], \bar{\mathbf{x}}, \mathbf{x}) &= \frac{1}{2} \sum_{i,j,k,h=1}^3 \frac{1}{\|\bar{\mathbf{x}} - \mathbf{x}\|^2} \alpha(\|\bar{\mathbf{x}} - \mathbf{x}\|) \lambda_{ijkh} \left(\|\bar{\mathbf{x}} - \mathbf{x}\| [\mathbf{e}^{(1)}(\bar{\mathbf{x}})]_{kh} + \mathcal{O}(\|\bar{\mathbf{x}} - \mathbf{x}\|^2) \right) \\ &\quad \times \left(\|\bar{\mathbf{x}} - \mathbf{x}\| [\mathbf{e}^{(1)}(\mathbf{x})]_{ij} + \mathcal{O}(\|\bar{\mathbf{x}} - \mathbf{x}\|^2) \right). \end{aligned} \quad (61)$$

Neglecting $\mathcal{O}(\|\bar{\mathbf{x}} - \mathbf{x}\|^2)$, then

$$\varphi([\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})], \bar{\mathbf{x}}, \mathbf{x}) \approx \frac{1}{2} \sum_{i,j,k,h=1}^3 \alpha(\|\bar{\mathbf{x}} - \mathbf{x}\|) \lambda_{ijkh} [\mathbf{e}^{(1)}(\bar{\mathbf{x}})]_{kh} [\mathbf{e}^{(1)}(\mathbf{x})]_{ij}. \quad (62)$$

Under the hypothesis of small deformations, $[\boldsymbol{\varepsilon}(\mathbf{x})]$ approximates $[\mathbf{e}^{(1)}(\mathbf{x})]$ and Eq. (62) is reduced to Eq. (48).

ii) If $\bar{\mathbf{x}} = \mathbf{x}$, then $[\Delta \mathbf{e}(\mathbf{x}, \mathbf{x}, \mathbf{0})]_{ij} = 0$. Hence, taking into account the polynomial decomposition of $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ (see Eq. (35)), it can be seen that Eq. (58) is reduced to Eq. (48) under the hypothesis of small deformations.

3.4 The Principle of Virtual Work in the Proposed Nonlocal Theory

Let $\mathbf{x} \mapsto \mathbf{u}(\mathbf{x})$ be the displacement field defined by $\mathbf{u}(\mathbf{x}) = \mathbf{r}(\mathbf{x}) - \mathbf{x}$. Let $\mathcal{C}_{\mathbf{u}}$ representing the set of admissible displacement fields satisfying the Dirichlet conditions on $\partial\Omega_0 \subset \partial\Omega$. Let $\mathcal{C}_{\delta\mathbf{u}}$ be the space of the test functions for which the Dirichlet conditions on $\partial\Omega_0$ are zero. To explicitly represent the functional dependency of $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ on \mathbf{u} , we introduce the tensor $\boldsymbol{\epsilon}$ such that $[\boldsymbol{\epsilon}(\mathbf{u}, \bar{\mathbf{x}}, \mathbf{x})] = [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$. The principle of virtual work, within the framework of the proposed theory, is written, for $\mathbf{u} \in \mathcal{C}_{\mathbf{u}}$, as

$$\int_{\Omega} \int_{\Omega} \sum_{i,j=1}^3 \frac{\partial \varphi([\boldsymbol{\epsilon}(\mathbf{u}, \bar{\mathbf{x}}, \mathbf{x})], \bar{\mathbf{x}}, \mathbf{x})}{\partial [\boldsymbol{\epsilon}(\mathbf{u}, \bar{\mathbf{x}}, \mathbf{x})]_{ij}} \delta [\boldsymbol{\epsilon}(\mathbf{u}, \bar{\mathbf{x}}, \mathbf{x}; \delta\mathbf{u})]_{ij} d\bar{\mathbf{x}} d\mathbf{x} = \delta \pi^{\text{ext}}(\mathbf{u}; \delta\mathbf{u}) \quad , \quad \forall \delta\mathbf{u} \in \mathcal{C}_{\delta\mathbf{u}}, \quad (63)$$

where φ is the deformation energy density defined by Eq. (53) and π^{ext} denotes the functional of external work. Since $[\boldsymbol{\epsilon}(\mathbf{u}, \bar{\mathbf{x}}, \mathbf{x})]$ is a functional of the N -th order derivatives of the displacement field \mathbf{u} , externally applicable loads are not just forces per unit volume and/or per unit area. The proposed model enables us to consider *external N -th order forces*, which refer to external actions that arise as dual to the work of the normal gradients of virtual displacements at the boundaries of the continuum, including its faces, edges, and wedges (see [50, 51, 52] related to 3rd and N -th gradient continua). We defer the deterministic and stochastic algebraic calculation of the equilibrium equations to future works.

4 Conclusions

In this paper, a higher-order nonlocal continuum model has been introduced for describing particle-based materials within a deterministic framework. [This paper, focusing on deterministic aspects, is the first part of a broader work. The subsequent part will address stochastic aspects within the framework of particle-based materials, considering uncertainties. Based on a novel pairwise deformation tensor that would correspond to the Green-Lagrange tensor in a nonlocal framework,](#) the proposed model offers two key advantages. First, it covers interactions over a longer range in comparison to those accounted for in the Eringen nonlocal elasticity. Second, it enables us to address complex external and contact actions, such as N -th order forces and stresses. This capability is analogous to the Piola peridynamics and N -th gradient continua. [Possible applications concern colloidal gels and colloidal crystals, whose significance in literature is growing thanks to their use in material science, biomedical engineering, optic, and 3D printing](#)

technology. Note that among the theoretical results presented in this paper, the orientation-preserving condition and Piola formula have been formulated in a nonlocal framework. A work, in progress, is devoted to the stochastic identification of the involved mechanical properties and interaction length for the anisotropic case. Finally, since the computational problem just requires the minimization of an energy functional, a weaker form could be introduced within the framework of Distribution Theory (also called Theory of Generalized Functions) to consider discontinuities such as those induced by fracture modeling. Furthermore, note that the proposed model can help in finding more general pairwise interactions resulting in N -th gradient continua, which can be useful for designing novel architected metamaterials.

Declarations

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Appendix

In this appendix, we give some of the formulas presented in this paper for $N = 2$, *i.e.*, for 2-nd gradient continua. In the following, summation is implied for repeated indices. Let us assume that \mathbf{r} at the point $\bar{\mathbf{x}}$ can be approximated using its Taylor expansion in the neighborhood of \mathbf{x} truncated at the second order,

$$r_i(\bar{\mathbf{x}}) = r_i(\mathbf{x}) + \frac{\partial r_i(\mathbf{x})}{\partial x_j}(\bar{x}_j - x_j) + \frac{1}{2} \frac{\partial^2 r_i(\mathbf{x})}{\partial x_j \partial x_k}(\bar{x}_j - x_j)(\bar{x}_k - x_k). \quad (64)$$

Let us define the tensor $\mathbf{f}^{(1)}(\mathbf{x})$ represented by the matrix $[\mathbf{f}^{(1)}(\mathbf{x})]$ such that

$$[\mathbf{f}^{(1)}(\mathbf{x})]_{ij} = \frac{\partial r_i(\mathbf{x})}{\partial x_j}. \quad (65)$$

The tensor $\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})$ represented by the matrix $[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]$ (see Eq. (5)) becomes

$$[\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]_{ij} = [\mathbf{f}^{(1)}(\mathbf{x})]_{ij} + \frac{1}{2} \frac{\partial [\mathbf{f}^{(1)}(\mathbf{x})]_{ij}}{\partial x_k}(\bar{x}_k - x_k). \quad (66)$$

Taking into account Eq. (65) and (66), Eq. (64) can be rewritten as

$$r_i(\bar{\mathbf{x}}) = r_i(\mathbf{x}) + [\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})]_{ij}(\bar{x}_j - x_j), \quad (67)$$

where $\det(\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x})) > 0$ under the hypothesis of orientation-preserving deformations. By taking into account Eq. (66), tensor $\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})$ represented by the matrix $[\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})]$ (see Eq. (12)) can be written in terms of components as

$$[\mathbf{c}(\bar{\mathbf{x}}, \mathbf{x})]_{pq} = [\mathbf{c}^{(1)}(\mathbf{x})]_{pq} + \frac{1}{2} c_{pqj}^{(12)}(\mathbf{x})(\bar{x}_j - x_j) + \frac{1}{4} c_{pqjk}^{(2)}(\mathbf{x})(\bar{x}_j - x_j)(\bar{x}_k - x_k), \quad (68)$$

where $\mathbf{c}^{(1)}(\mathbf{x})$ is the right Cauchy-Green tensor (see Eq. (32)), $\mathbf{c}^{(12)}(\mathbf{x}) = \nabla \mathbf{c}^{(1)}(\mathbf{x})$ is the third-order tensor whose components are

$$c_{pqj}^{(12)}(\mathbf{x}) = [\mathbf{f}^{(1)}(\mathbf{x})]_{ip} \frac{\partial [\mathbf{f}^{(1)}(\mathbf{x})]_{iq}}{\partial x_j} + \frac{\partial [\mathbf{f}^{(1)}(\mathbf{x})]_{ip}}{\partial x_j} [\mathbf{f}^{(1)}(\mathbf{x})]_{iq}, \quad (69)$$

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

$$c_{pqjk}^{(2)}(\mathbf{x}) = \frac{\partial [\mathbf{f}^{(1)}(\mathbf{x})]_{ip}}{\partial x_j} \frac{\partial [\mathbf{f}^{(1)}(\mathbf{x})]_{iq}}{\partial x_k}. \quad (70)$$

Taking into account Eq. (68), tensor $\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})$ represented by the matrix $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ (see (14)) can be rewritten in terms of components as

$$[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]_{pq} = [\mathbf{e}^{(1)}(\mathbf{x})]_{pq} + \frac{1}{4} c_{pqj}^{(12)}(\mathbf{x})(\bar{x}_j - x_j) + \frac{1}{8} c_{pqjk}^{(2)}(\mathbf{x})(\bar{x}_j - x_j)(\bar{x}_k - x_k). \quad (71)$$

Deriving Eq. (64) with respect to $\bar{\mathbf{x}}$, it is not difficult to show that $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] = [\mathbf{e}(\mathbf{x}, \bar{\mathbf{x}})]$ and, consequently, $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})] = [\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$. Thus, replacing Eq. (71) into Eq. (53), we obtain a novel deformation energy density suitable for particle-based materials under the hypothesis of 2-nd gradient continua. Further details and computational aspects will be addressed in the second part of the paper. It will be shown that tensor $[\mathbf{e}(\bar{\mathbf{x}}, \mathbf{x})]$ allows us to formulate even more general models, exploring the possibility to encompass gradient-type and integral nonlocal theories.

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