

# Computational method for mapping continuum deformations to crystal lattices containing defects

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## Abstract

Computational multiscale methods that perform concurrent simulations of atoms and solid continua generally rely on classical assumptions for kinematics, such as the Cauchy-Born approximation, for deformations of perfect crystals. For the treatment of crystal defects, such assumptions do not apply and one is left only with performing full-scale atomistic energy minimizations. We present interim progress on an approach based on homogenization to enable continuum notions of deformations to apply to defected lattices. Using a decompositional kinematical representation, we present a single parameter line search method for the minimization procedure, with the intent of substantially reducing the computational cost.

*Keywords:* Multiscale; Finite elements; Atomistics; Plasticity; Large deformation

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## 1. Introduction

The rational approach for treating deforming crystals is to apply continuum deformation quantities, such as the the deformation gradient, to atomic vector and tensorial variables. This way of mapping deformations is classically due to Cauchy [1] and later to Born [2]. For perfect, defect-free systems this type of mapping has been shown to ably represent the correct configurations [3] even for complex lattice deformations such as twins [4]. However, the Cauchy and Born assumptions are not without limitations when considering physical phenomenology such as lattice instabilities [5]. But for most applications and numerical methods [6] the assumptions have yielded successful multiscale calculations.

Unfortunately, materials with localized point or edge defects are fundamentally inconsistent with the assumptions of Cauchy and Born, even for small strain elasticity. Existing numerical methods therefore rely on full atomic scale minimizations to handle anharmonic crystal regions. The continuum, therefore, is inherently assumed to be a perfect lattice and distributed networks of defects more representative of realistic engineering materials would therefore be prohibitive or intractable. With increasing interest in solid mechanics with full

atomic resolution, it is desirable to have methods that can accurately capture defect mechanisms without having to perform full minimizations of the atoms. In an effort to increase engineering utility and realism, we extend an earlier homogenization method [7, 8] based on a single parameter minimization procedure while incorporating finite deformation concepts to handle larger classes of atomic-to-continuum multiscale problems.

## 2. Preliminaries

The kinematics and constitutive definitions are defined in the standard way. Let us assume that a body  $\mathcal{B} \subset \mathbb{R}^3$  has points  $\mathbf{X} \in \mathcal{B}$  in regular cartesian space (with respect to the coordinate base  $\mathbf{E}$ ) that get mapped to points  $\mathbf{x} \in \mathcal{S}$  (coordinate base  $\mathbf{e}$ ) through  $\phi(X, t) : \mathcal{B} \rightarrow \mathcal{S}$ . At the moment, we only assume  $\phi$  to be *at least*  $C^1$ , or that it is differentiable at least once. In the context of lattice and atomistic mechanics, this presupposes that all considerations are for diffusionless mechanisms. This tight restriction is assumed throughout our developments. In the numerical implementation, however, this restriction is relaxed and only loosely enforced by invoking an incremental procedure.

The deformation gradient  $\mathbf{F}$  is formally defined as the mapping of tangent bundles in  $\mathcal{B}$  or, stated differently, the tangent of  $\phi$ ,  $\mathbf{F} = T\phi$ . In order to use this point

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mapping, one must supply a restriction of  $\mathbf{F}$  to a tangent on  $\mathcal{B}$  at a point  $\mathbf{X}$ . Namely:

$$\mathbf{F}(X) = (\mathbf{F})_A^a(X) = \frac{\partial \phi^a}{\partial X^A}(X) \quad (1)$$

The Green deformation tensor is defined as

$$\mathbf{C} = \mathbf{F}^T \mathbf{F} \quad (2)$$

or in indicial form

$$C^{AB} = (\mathbf{F}^T)_a^A F_B^a \quad (3)$$

which is symmetric and positive definite. To complete the preliminary kinematical definitions, we define the rate of deformation tensor  $\mathbf{D}$  as:

$$\mathbf{D}(X,t) = \frac{\partial}{\partial t} \mathbf{C}(X,t) \quad (4)$$

As is customary for the definition of a stress and, in particular, the Cauchy stress we first assume the existence of a vector field  $\mathbf{t}(x, t, \mathbf{n})$ , called the Cauchy stress vector, where  $x$  specifies its position in space,  $t$  its position in time and  $\mathbf{n}$  its orientation. It physically represents the force per unit area exerted on a surface element, whether a fictitious surface within a body or the bounding surface of the body itself, oriented normal to  $\mathbf{n}$ . It can subsequently be shown that there is a second-order tensor field  $\boldsymbol{\sigma}$  defined by:

$$\mathbf{t}(x,t, \mathbf{n}) = \boldsymbol{\sigma}(x,t) \cdot \mathbf{n} = \langle \boldsymbol{\sigma}(x,t), \mathbf{n} \rangle \quad (5)$$

where the definition of the vector inner product is also shown. The tensor  $\boldsymbol{\sigma}$  is called the Cauchy stress tensor. In indicial form, we may write:

$$t^a(x,t, \mathbf{n}) = \sigma^{ac}(x,t) g_{bc} n^b = \sigma_b^a n^b \quad (6)$$

From here, we also define the first Piola-Kirchhoff stress tensor as:

$$P^{aA} = J(\mathbf{F}^{-1})_b^A \sigma^{ab} \quad (7)$$

and the second Piola-Kirchhoff stress tensor as:

$$S^{AB} = (F^{-1})_b^A P^{aB} = J(\mathbf{F}^{-1})_b^A (\mathbf{F}^{-1})_c^B \sigma^{ab} \quad (8)$$

We next assume the existence of an identifiable free energy function  $\Psi$ . We assume an underlying theory of hyperelasticity in the manner of Marsden and Hughes [9] and begin with the conventional equations of Lagrangian continuum mechanics. This entails the following set of equations:

$$\rho_o = \rho J \quad (9)$$

$$\rho_o \frac{d\mathbf{V}}{dt} = \text{DIV} \mathbf{P} + \rho_o \mathbf{B} \quad (10)$$

$$\mathbf{S} = \mathbf{S}^T \quad (11)$$

$$\rho_o \frac{\partial E}{\partial t} + \text{DIV} \mathbf{Q} = \rho_o R + \mathbf{S} : \mathbf{D} \quad (12)$$

$$\rho_o N \frac{\partial \Theta}{\partial t} + \frac{\partial \Psi}{\partial t} - \mathbf{S} : \mathbf{D} + \frac{1}{\Theta} \langle \mathbf{Q}, \text{GRAD} \Theta \rangle \leq 0 \quad (13)$$

$$E = \Psi + N \Theta \quad (14)$$

where  $\rho$  and  $\rho_o$  are the respective spatial and material densities,  $\mathbf{V}$  is the material velocity,  $\text{DIV}$  is the divergence operator in the material frame,  $\mathbf{P}$  is the first Piola-Kirchhoff stress,  $N$  is the entropy,  $\mathbf{S}$  is the second Piola-Kirchhoff stress,  $E$  is the internal energy density per unit mass,  $\mathbf{Q}$  is the material heat flux vector,  $R$  is the internal power generated per unit mass,  $\mathbf{D}$  is the rate of deformation tensor,  $\Psi$  is the free energy,  $\Theta$  is the absolute temperature, and the operator  $d/dt$  is the material derivative defined by:

$$\frac{d\mathbf{V}}{dt} = \frac{dV^a}{dt} = \frac{\partial V^a}{\partial t} + \gamma_{bc}^a V^b V^c \quad (15)$$

where  $\gamma$  is a Christoffel symbol for the Riemann metric  $\mathbf{g}$  in the spatial configuration.

Equation (9) is the equation of mass conservation where  $J$  is the Jacobian relating the original to current volume. Equation (10) is the conservation of linear momentum equation involving the material derivative in Eq. (15) due to the Lagrangian framework. The symmetry of the stress tensor is assured by the conservation of angular momentum in Eq. (11). The energy balance is given in Eq. (12). The thermodynamic laws are satisfied through the inequation in Eq. (13) and the definition for internal energy in Eq. (14).

In the absence of temperature effects the free energy is exactly equal to the stored energy function  $W$ . In this discussion, however, we will maintain generality by assuming nonisothermal conditions. However, where convenient, we will remove this general treatment in favor of the simpler isothermal (or even zero temperature) case.

With the assumption of an existing free energy function,  $\Psi$ , the stress tensors may be given by:

$$\boldsymbol{\sigma} = 2\rho \frac{\partial \Psi}{\partial \mathbf{g}} \quad (16)$$

$$\mathbf{P} = \rho_o \frac{\partial \Psi}{\partial \mathbf{F}} \quad (17)$$

$$\mathbf{S} = 2\rho_o \frac{\partial \Psi}{\partial \mathbf{C}} \quad (18)$$

where we have taken some liberties in a nonrigorous definition of functional dependencies in  $\Psi$ , namely that  $\Psi$  can be a function of  $\mathbf{g}$ ,  $\mathbf{F}$  or  $\mathbf{C}$  interchangeably with some modification. The indicial counterparts of these forms are given by:

$$\sigma^{ab} = 2\rho \frac{\partial \Psi}{\partial g_{ab}} \quad (19)$$

$$P_a^A = \rho_o \frac{\partial \Psi}{\partial F_A^a} \quad (20)$$

$$S^{AB} = 2\rho_o \frac{\partial \Psi}{\partial C_{AB}} \quad (21)$$

As the current developments are based on fundamental principles stemming from the invocation of an incremental numerical implementation (to be discussed later), the material property tensors can be viewed as tangents of the actual nonlinear material. Insofar as hyperelasticity applies to the classes of problems in which we are interested, we may write the elasticity tensors in the following way<sup>1</sup>. Let us assume that  $\mathbf{P}$  and  $\mathbf{S}$  are used in the functional forms of Eqs. (7) and (8), respectively, that is, that they have functional dependence on some kinematic variable. Then the first and second elasticity tensors are respectively defined as:

$$\mathcal{A} = \frac{\partial \mathbf{P}}{\partial \mathbf{F}}, \quad \mathcal{C} = \frac{\partial \mathbf{S}}{\partial \mathbf{C}} \quad (22)$$

or in indicial form:

$$\mathcal{A}_{aB}^{aA} = \frac{\partial P^{aA}}{\partial F_B^a}, \quad \mathcal{C}^{ABCD} = \frac{\partial S^{AB}}{\partial C_{CD}} \quad (23)$$

These may also be related to the free energy function  $\Psi$  by substituting Eqs. (17) and (18) (or 20 and 21) into Eqs. (22) (or 23) to obtain:

$$\mathcal{A}_{aB}^{aA} = \rho_o \frac{\partial^2 \Psi}{\partial F_A^a \partial F_B^a}, \quad \mathcal{C}^{ABCD} = 2\rho_o \frac{\partial^2 \Psi}{\partial C_{AB} \partial C_{CD}} \quad (24)$$

### 3. Classical kinematics

As our more immediate intent is to develop a kinematical mapping procedure for crystals containing a defect, we start with the classical mapping approximation used commonly for perfect single crystals – the so-called Born hypothesis. Originally due to Cauchy [1] and Born [2], the essential definition is as follows [4]. Given a reference multi-lattice  $\mathcal{L}$  with a corresponding Bravais lattice  $\mathcal{R}$  generated from lattice vectors  $\bar{\mathbf{E}}_I$ , the deformed Bravais lattice  $\mathcal{R}'$  due to deformation from an admissible macroscopic homogeneous gradient  $\mathbf{F} : \mathcal{R} \rightarrow \mathcal{R}'$  can be generated by lattice vectors  $\bar{\mathbf{E}}'_i$  such that:

$$\bar{\mathbf{E}}'_i = m_i^I \mathbf{F} \bar{\mathbf{E}}_I \quad (25)$$

where  $m_i^I$  is from the set of all invertible  $3 \times 3$  matrices with integer coefficients, i.e. this is the three-dimensional integer multiplier to generate the space filling crystal.

A more restrictive form of this rule, which we refer to as the Cauchy-Born rule, is often found in multiscale methods for complex multi-lattices [6, 10, 11] in which the motion of shift vectors  $p_k$  for  $k$  interpenetrating Bravais lattices, is also controlled in the deformation in addition to the primitive lattice vectors. This is denoted by saying that all points given by  $\mathbf{X} = m^I \bar{\mathbf{E}}_I + p_k$  with  $m^I$  being any integer maps point by point to  $\mathbf{x}$  such that:

$$\mathbf{x} = \mathbf{F}\mathbf{X} \quad (26)$$

As one may expect, in general, the range of strains in which Eq. (26) is applicable is significantly smaller than for Eq. (25) because of the additional constraint of the shift vectors.

### 4. Homogenization

At this point, we invoke the basic assumptions of simple two-scale asymptotic expansion homogenization [12], which are that two coordinate systems,  $\mathbf{X}$  and  $\mathbf{Y}$ , that have the same basis exist and that all variables defined in  $\mathbf{Y}$  are  $\mathbf{Y}$ -periodic. The ‘simple’ homogenization procedure is to assume an absence of finite rotations such that the spatial coordinate systems,  $\mathbf{x}$  and  $\mathbf{y}$ , can be defined with respect to the same material frame basis. In particular, we will look for functions  $\mathbf{u}^\epsilon$  which are the displacements, such that:

$$\mathbf{u}^\epsilon(\mathbf{x}, \mathbf{y}) = \mathbf{u}^{(0)}(\mathbf{x}) + \epsilon \mathbf{u}^{(1)}(\mathbf{x}, \mathbf{y}) + \epsilon^2 \mathbf{u}^{(2)}(\mathbf{x}, \mathbf{y}) + \dots \quad (27)$$

where  $\epsilon$  is the asymptotic scaling parameter,  $\mathbf{y} = \mathbf{x}/\epsilon$ . The finite rotation form of this derivation will be reserved for a later paper that will more carefully address arbitrary bases.

With our present assumption of simplicity, we may write the usual deformation gradient,  $\mathbf{F}$ , as:

$$\mathbf{F} = \mathbf{I} + \mathbf{H}^\epsilon \quad (28)$$

$$= \mathbf{I} + \nabla^\epsilon \mathbf{u}^\epsilon \quad (29)$$

$$= \mathbf{I} + \left( \nabla^X + \frac{1}{\epsilon} \nabla^Y \right) (\mathbf{u}^{(0)}(\mathbf{x}) + \epsilon \mathbf{u}^{(1)}(\mathbf{x}, \mathbf{y}) + \epsilon^2 \mathbf{u}^{(2)}(\mathbf{x}, \mathbf{y}) + \dots) \quad (30)$$

$$= \mathbf{I} + \mathbf{H}^{(0)} + \epsilon \mathbf{H}^{(1)} + \epsilon^2 \mathbf{H}^{(2)} + \dots \quad (31)$$

where  $\mathbf{I}$  is the second order identity tensor and

$$\mathbf{H}^{(n)} = \nabla^X \mathbf{u}^{(n)} + \nabla^Y \mathbf{u}^{(n+1)} \quad (32)$$

and the gradient operators are defined by  $\nabla^X = \partial/\partial \mathbf{X}$  and  $\nabla^Y = \partial/\partial \mathbf{Y}$ .

We now propose the following. If  $\bar{\mathbf{F}}$  is the minimizer of the free energy function  $\Psi$  and  $\bar{\mathbf{F}}^o$  is the Cauchy-Born

rule deformation gradient, then there exists a decomposition of  $\bar{\mathbf{F}}$  such that:

$$\bar{\mathbf{F}}(\mathbf{X}, \mathbf{Y}) = \bar{\mathbf{F}}^*(\mathbf{X}, \mathbf{Y}) \bar{\mathbf{F}}^o(\mathbf{X}). \quad (33)$$

The proof of Eq. (33) is in the remaining task of determining  $\bar{\mathbf{F}}^*$  with respect to our assumptions of homogenization. It also remains to define the appropriate computational method for determining each of the terms in Eq. (33) numerically.

Let us first remark that that other terms in Eq. (33) can be readily defined. The Cauchy-Born deformation gradient is defined ‘simply’ by:

$$\bar{\mathbf{F}}^o(\mathbf{X}) = \mathbf{I} + \nabla^X \mathbf{u}^{(0)}(\mathbf{x}) \quad (34)$$

The homogenization procedure of [7, 8] can be generalized for finite strain to obtain:

$$\bar{\mathbf{F}} = \mathbf{I} + \mathbf{H}^{(0)} \quad (35)$$

Combining these two results then readily leads to:

$$\begin{aligned} \bar{\mathbf{F}}^* &= (\bar{\mathbf{F}}^o)^{-1} \bar{\mathbf{F}} \\ &= \mathbf{I} + (\mathbf{I} + \nabla^X \mathbf{u}^{(0)})^{-1} \nabla^Y \mathbf{u}^{(1)} \end{aligned} \quad (36)$$

The generalization that leads to Eq. (35) will be detailed in the final conference paper. The procedure for obtaining  $\mathbf{u}^{(1)}$  has been shown in earlier related works [7].

The decomposition approach for multiscale applications have been considered before [13,14]. The basic idea presently used falls back to early thoughts on plasticity [15] of decomposing deformations that separates lattice slip from bulk motions. The point of departure in this work is that in deforming lattices containing defects, molecular motions, due to their high degree of non-linearity, undergo subsequent point-wise relaxations that we presume have a structure representable in some variational form. The minimization problem in the smaller of the two scales is essentially a harmonic extension of the atomistic problem, or the so-called ‘umbrella’ potential problem. The connection to distributed networks of defects is achieved through the simple Y-periodicity argument, which, at first, appears overly simplistic but remains powerful through subsequent computational developments.

Finally, we must also remark that the instantaneous harmonic assumption needed to get the result in Eq.(35) is non-trivial and restrictive. In fact, it can be shown that, owing to this caveat,  $\bar{\mathbf{F}}$  is not a true minimizer of  $\Psi$ . A better minimizer involves a scalar parameter  $\alpha$  such that

$$\bar{\mathbf{F}}(\mathbf{X}, \mathbf{Y}) = \alpha \bar{\mathbf{F}}^*(\mathbf{X}, \mathbf{Y}) \bar{\mathbf{F}}^o(\mathbf{X}) \quad (37)$$

which we present here without proof. Therefore, the

nonlinear multibody atomistic problem is now replaced by a linear minimization of the harmonic equations *plus* a single parameter line search.

## Notes

<sup>1</sup>In general, the connection to atomistics is precarious since much remains to be said for the substitution of an atomistic functional in place of the free energy  $\Psi$ , in part or in whole, and the interpretation of  $\mathbf{t}$  as atomic forces per unit area. However, we can still meaningfully use tangent stiffnesses obtained from derivatives of the atomistic ‘free energy’ since one can show locality and invariance properties are generally satisfied for these potentials in a crystallographic sense. One can also show that for zero temperature molecular statics/dynamics and finite temperature dynamics, either as trajectory simulations or quasi-static quenching simulations, the second thermodynamic law is satisfied. In fact, p. 191 of Marsden and Hughes [9] proves that by using hyperelastic constitutive laws we can implicitly assume this.

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