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CONFIGURATIONAL FORCES INDUCED BY FINITE-ELEMENT DISCRETIZATION

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Abstract. In standard finite-element analysis a fixed mesh is prescribed in the undeformed body and the strain energy is considered as a function of nodal displacements. Since the strain energy also depends inherently on the prescribed nodal coordinates of the mesh, any shift of a node in the undeformed body will cause a change of strain energy in the deformed state. This gives rise to the definition of configurational forces acting on the nodes in the undeformed body. The forces are represented in terms of the Eshelby stress tensor. The undeformed finite-element mesh can be modified such as to make the inner configurational forces vanish. Only the boundary nodes have to sustain configurational forces normal to the boundary, to preserve the shape of the body.

Key words: inhomogeneities, configurational forces, the Eshelby stress tensor, finite elements.

1. INTRODUCTION

The concept of a force acting on a geometrical singularity within an elastic body has been introduced, decades ago, by Eshelby [1]. Configurational forces, in general, are those forces which are exerted on any kind of imperfection such as dislocations, disclinations, inclusions, voids, etc. by the surrounding continuum. In the context of dynamics configurational forces have been studied in the recent years by Maugin [2].

The static deformation of an elastic solid is described, as in [3], by functions

$$x^i = x^i(X^I) \tag{1.1}$$

relating the coordinates x^i of the actual position of a material point to the coordinates X^I of its position in the stress-free reference state. The strain-energy density, per unit volume of the undeformed material, is a function

$$W = W(x^i{}_{,I}, X^K) \tag{1.2}$$

depending on the deformation gradient $x^i{}_{,I} \equiv \partial x^i / \partial X^I$ and, in the case of an inhomogeneous material, also directly on the material coordinates X^K. The constitutive equation (1.2) has to meet the requirements of material frame indifference and to reflect the symmetry properties of the material.

The first Piola–Kirchhoff stress tensor is obtained from the strain-energy density by

$$T_i{}^I = \frac{\partial W}{\partial x^i{}_{,I}}. \tag{1.3}$$

It delivers the stress in the actual placement acting on a surface element specified in the reference placement. A material region $\mathcal{B}_X$ marked off in the reference placement is exposed in the actual placement to the total force

$$f_i = \int_{\partial \mathcal{B}_X} T_i{}^J \, \mathrm{d}A_J \tag{1.4}$$

by the surrounding material. This is a physical, or Newtonian, force as opposed to the configurational force introduced below.

Eshelby's original reasoning is sketched briefly as follows. Into a stress-free elastic body an unspecified defect is inserted at some location inside a region $\mathcal{B}_X$ (Fig. 1). Due to the defect the whole body undergoes a deformation, especially the region $\mathcal{B}_X$ is deformed to $\mathcal{B}_x$. The same procedure is repeated with an identical replica of the body, in which the marked-off region is shifted by a small vector $-\delta X^I$ such that the shifted region $\mathcal{B}'_X$ still contains the defect. Now the region $\mathcal{B}_x$ is cut out from the deformed original body and replaced by $\mathcal{B}'_x$ from the deformed replica. Since the deformed regions $\mathcal{B}_x$ and $\mathcal{B}'_x$ are not congruent any more, appropriate self-equilibrating forces have to be applied on their boundaries before they can be glued together. When the whole procedure is finished, the defect has been shifted by the vector $+\delta X^I$ relative to the undeformed body. Reckoning up the energy change and expenditure of work during this hypothetical process, one obtains a net change of total energy, as if one had to work against a force while shifting the defect. This configurational force can be calculated from the Eshelby stress tensor

$$\mathcal{E}_I{}^J = W \delta_I^J - x^i{}_{,I} \, T_i{}^J \tag{1.5}$$

by integration around the boundary $\partial \mathcal{B}_X$ containing the defect:

$$\mathcal{F}_I = \int_{\partial \mathcal{B}_X} \mathcal{E}_I{}^J \, \mathrm{d}A_J \, . \tag{1.6}$$

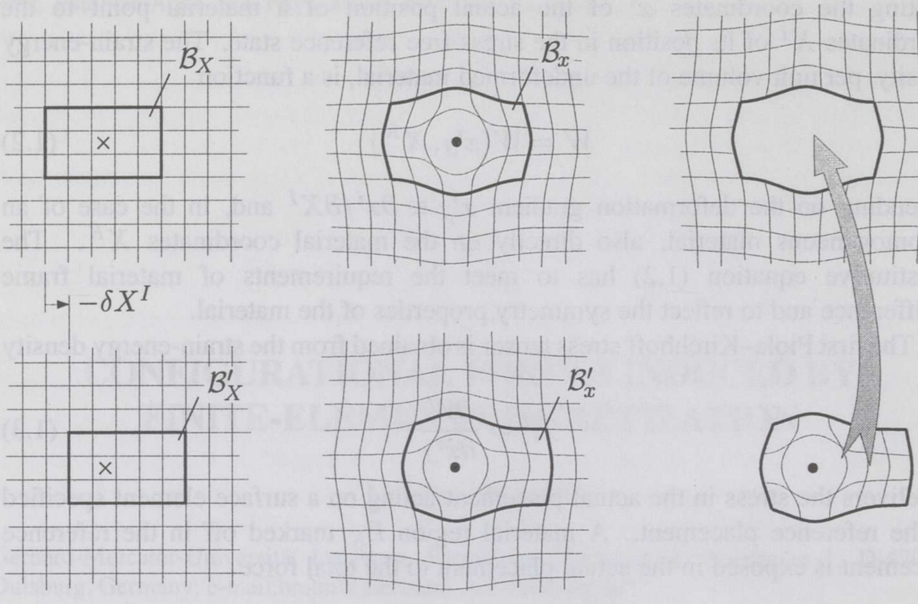

Fig. 1. Eshelby's concept of a force acting on a defect.

Actually Eshelby's original "energy-momentum" tensor differs from (1.5) by a divergence-free term and leads to the same force (1.6). The formulation presented here is more appropriate for finite deformations.

An explicit calculation of the configurational force (1.6) in closed form will not be possible in most cases. A numerical approach, however, is quite convenient, since all the ingredients of the Eshelby stress tensor (1.5) are provided by a finite-element calculation. As a simple test example one can calculate the configurational force exerted on a region that does not contain any defect. The finite-element method will predict a nonzero force, in general, although it should vanish. This effect will be analysed in the sequel.

2. FINITE ELEMENTS

The finite-element method approximates the deformation (1.1) by interpolation or shape functions, which are specified within each of the elements by certain nodal variables. More specifically, the deformation $x^i = x^i(X^I)$ is not attacked directly. Instead, the coordinates X^I and x^i are considered as functions of a new set of parameters ξ^α. These can be interpreted as the coordinates in a certain standard form of the element. For instance, every triangular element is generated from a right-angled isosceles prototype, in which all the necessary calculations are performed (Fig. 2). This prototype is mapped to the reference placement by a transformation

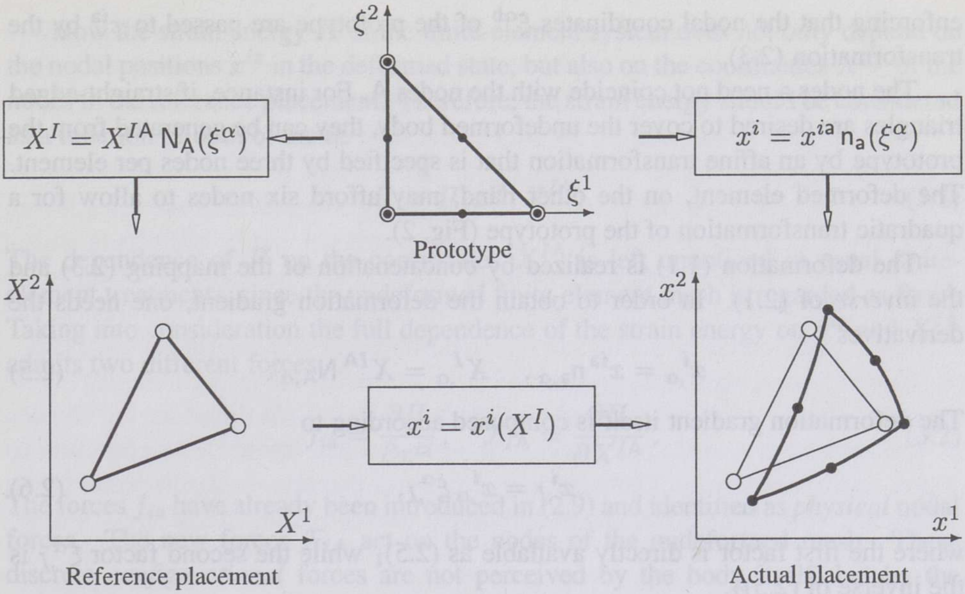

Fig. 2. Placements of a triangular finite element.

$$X^I = X^I(\xi^\alpha) = X^{IA}\,\mathsf{N_A}(\xi^\alpha)\,, \tag{2.1}$$

which depends on the coordinates X^{IA} of the nodes A in the reference placement. Since the nodal coordinates $\xi^{\alpha A}$ of the prototype must be mapped into the prescribed nodal coordinates X^{IA} of the reference placement, the corresponding shape functions $\mathsf{N_A}(\xi^\alpha)$ have to satisfy the condition

$$\mathsf{N_A}(\xi^{\alpha B}) = \delta^{B}_{A}\,. \tag{2.2}$$

The map (2.1) does not describe an actual deformation of the elastic body. It serves only to adjust shape and size of a certain finite element to fit into the chosen element net.

The same prototype is now mapped to the actual placement, thus representing the deformed version of the element. The corresponding transformation is

$$x^i = x^i(\xi^\alpha) = x^{ia}\,\mathsf{n_a}(\xi^\alpha) \tag{2.3}$$

with x^{ia} denoting the coordinates of the nodes in their actual position. In contrast to the prescribed coordinates X^{IA}, the nodal coordinates x^{ia} are unknown, in general, with possible exception of some nodes fixed by supports. Again, the shape functions $\mathsf{n_a}(\xi^\alpha)$ have to satisfy the characteristic condition

$$\mathsf{n_a}(\xi^{\alpha b}) = \delta^{b}_{a}\,, \tag{2.4}$$

enforcing that the nodal coordinates $\xi^{\alpha \mathsf{b}}$ of the prototype are passed to $x^{i\mathsf{a}}$ by the transformation (2.3).

The nodes a need not coincide with the nodes A. For instance, if straight-edged triangles are desired to cover the undeformed body, they can be generated from the prototype by an affine transformation that is specified by three nodes per element. The deformed element, on the other hand, may afford six nodes to allow for a quadratic transformation of the prototype (Fig. 2).

The deformation (1.1) is realized by concatenation of the mapping (2.3) and the *inverse* of (2.1). In order to obtain the deformation gradient, one needs the derivatives

$$x^i{}_{,\alpha} = x^{i\mathsf{a}}\, \mathsf{n}_{\mathsf{a},\alpha}\,, \qquad X^I{}_{,\alpha} = X^{I\mathsf{A}}\, \mathsf{N}_{\mathsf{A},\alpha}\,. \tag{2.5}$$

The deformation gradient itself is composed according to

$$x^i{}_{,I} = x^i{}_{,\alpha}\, \xi^\alpha{}_{,I}, \tag{2.6}$$

where the first factor is directly available as $(2.5)_1$ while the second factor $\xi^\alpha{}_{,I}$ is the inverse of $(2.5)_2$.

In a homogeneous elastic material the strain-energy density W depends only on the deformation gradient. The total strain energy is

$$\Pi = \int_{\mathcal{B}_\xi} W(x^i{}_{,\alpha}\, \xi^\alpha{}_{,I})\, J\, \mathrm{d}V_\xi\,, \tag{2.7}$$

where the integration is performed over the prototype region $\mathcal{B}_\xi$ and

$$J = \det(X^I{}_{,\alpha}) \tag{2.8}$$

denotes the Jacobian of the map (2.1). The strain energy of the elastic body is now considered as a function $\Pi = \Pi(x^{i\mathsf{a}})$ depending on the actual positions $x^{i\mathsf{a}}$ of the nodes. The derivative

$$\frac{\partial \Pi}{\partial x^{i\mathsf{a}}} = f_{i\mathsf{a}} \tag{2.9}$$

yields the external nodal forces. The finite-element computation has to solve the system of equations (2.9) for the unknown nodal positions $x^{i\mathsf{a}}$ when the external nodal forces $f_{i\mathsf{a}}$ are given. For nonlinear problems this can be done only by iteration.

3. PHYSICAL AND CONFIGURATIONAL FORCES

The nodal forces $f_{i\mathsf{a}}$ are physical or Newtonian forces exerted on discrete points of the body. They are discrete approximations to the actual forces, which are continuously distributed over the volume and the boundary. But this does not detract from their physical nature.

Now the strain energy Π of the finite-element system does not only depend on the nodal positions x^{ia} in the deformed state, but also on the coordinates X^{IA} of the nodes in the reference placement. Therefore, the strain energy should be considered as a function of both of them:

$$\Pi = \Pi(x^{ia}, X^{IA}). \tag{3.1}$$

The dependence of Π on the coordinates X^{IA} is left unnoticed in usual finite-element treatments, since the undeformed finite-element mesh is regarded as fixed. Taking into consideration the full dependence of the strain energy on x^{ia} and X^{IA} admits two different forces

$$f_{ia} = \frac{\partial \Pi}{\partial x^{ia}}, \quad \mathcal{F}_{IA} = \frac{\partial \Pi}{\partial X^{IA}}. \tag{3.2}$$

The forces f_{ia} have already been introduced in (2.9) and identified as *physical* nodal forces. The new forces $\mathcal{F}_{IA}$ act on the nodes of the undeformed mesh. These discrete *configurational* forces are not perceived by the body itself, but by the agency prescribing the nodes in the undeformed body.

In order to obtain explicit expressions for the two kinds of forces (3.2), one has just to trace the dependences of the strain energy (2.7) upon the two kinds of nodal coordinates. The coordinates x^{ia} of the actual nodal position enter via the factor $x^i{}_{,\alpha}$ of the deformation gradient, which is the argument of the strain-energy density. Using (1.3) and $(2.5)_1$, one obtains immediately

$$f_{ia} = \int_{\mathcal{B}_\xi} T_i{}^I \, \mathsf{N}_{a,I} \, J \, \mathrm{d}V_\xi \,. \tag{3.3}$$

The nodal coordinates X^{IA}, occurring directly in $(2.5)_2$, are hidden at two places within the integral (2.7): Both the Jacobian J and the inverse derivative $\xi^\alpha{}_{,I}$ depend indirectly on the coordinates X^{IA}. According to well-known formulas of tensor analysis, we have

$$\frac{\partial J}{\partial X^{IA}} = J \, \mathsf{N}_{A,I} \,, \quad \frac{\partial \xi^\alpha{}_{,J}}{\partial X^{IA}} = -\xi^\alpha{}_{,I} \, \mathsf{N}_{A,J} \,. \tag{3.4}$$

Using these derivatives, the configurational nodal force can be expressed in terms of the Eshelby stress tensor (1.5) by

$$\mathcal{F}_{IA} = \int_{\mathcal{B}_\xi} \mathcal{E}_I{}^J \, \mathsf{N}_{A,J} \, J \, \mathrm{d}V_\xi \,. \tag{3.5}$$

Thus, the configurational nodal force is obtained from the Eshelby stress tensor in the same way as the physical nodal force (3.3) is generated by the Piola–Kirchhoff stress tensor.

The domain of integration $\mathcal{B}_\xi$ in (3.3) and (3.5) represents a collection of prototype elements, from which the finite-element mesh covering the whole body is generated. But only those elements contribute to the integral, which are adjacent to the considered node, since otherwise the derivatives of the shape functions vanish. Therefore it suffices to integrate over the elements surrounding the node.

For the body as a whole the physical nodal forces are due to the external loads. If these are applied only on the boundary, the inner nodes are free of *physical* nodal forces. *Configurational* nodal forces, however, are present at all nodes, in general. This suggests the question, whether a finite-element net can be tailored in such a way that the configurational forces vanish. To preserve the shape of the body the boundary nodes should be kept fixed or at least confined to the fixed boundary. But the inner nodes could be released to take a position free of configurational forces.

Figure 3 shows a simple problem of plane elasticity, solved by triangular finite elements. In the left picture a fixed mesh is prescribed. Then the nodes are allowed to float into new positions, shown in the right picture, where the configurational forces are (nearly) zero. The boundary nodes still perceive configurational forces which are normal to the boundary and prevent the body from shrinking.

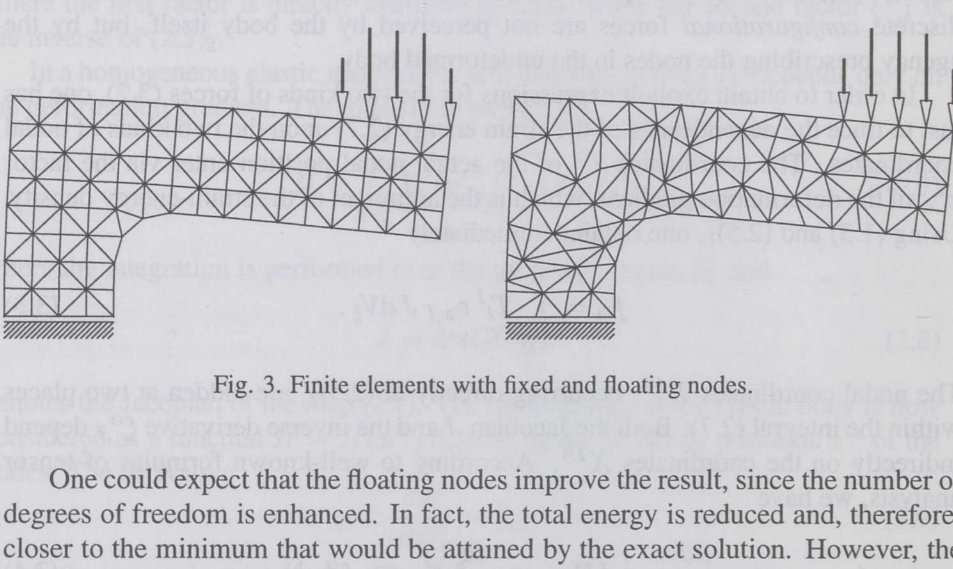

Fig. 3. Finite elements with fixed and floating nodes.

One could expect that the floating nodes improve the result, since the number of degrees of freedom is enhanced. In fact, the total energy is reduced and, therefore, closer to the minimum that would be attained by the exact solution. However, the new mesh contains several bad-shaped elements, which make it worse than the original mesh from the numerical point of view. As long as the topological structure of the mesh is kept fixed, the variation of nodes will not necessarily improve a finite-element solution.

4. CONCLUSIONS

Discrete configurational forces are always anchored at inherent irregularities within an otherwise homogeneous continuum. They are not restricted to real defects within a material, such as inclusions, voids, cracks, dislocations, and disclinations, but may also be tied to artificial substructures that are introduced by numerical discretization. The spurious configurational forces induced by a finite-element net have been analysed in detail.

The strain energy of an elastic body, in its finite-element approximation, is regarded as a function of the nodal coordinates in both the deformed and the undeformed mesh. The corresponding derivatives of this strain-energy function yield two different types of nodal forces, the physical and the configurational forces. The latter are not really perceived by the material. Rather they indicate the change of energy that is generated by the shift of a node in the undeformed mesh. The configurational nodal forces are expressed in terms of the Eshelby stress tensor.

The undeformed mesh can be modified such as to make the configurational forces at internal nodes vanish. Such a mesh stands out for minimum total energy when compared with other meshes of the same topological connectivity. A substantial improvement, however, should admit also changes of the topology, which would be accompanied by "quantum jumps" of the energy. This lies outside the scope of configurational forces.

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LÕPLIKE ELEMENTIDE DISKREETSUSEST PÕHJUSTATUD KUJUJÕUDUDEST

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Standardse lõplike elementide meetodi kasutamisel seotakse elemendid deformeerumata kehaga ja vaba energia on sõlmede siirete funktsioon. Elementide valiku muutumisel teiseneb ka vaba energia, mis võib olla väljendatud kujujõudude abil. Käesolevas artiklis on esitatud kujujõud Eshelby pingetensori abil ja näidatud, missugune peab olema sõlmede valik, et sisesõlmedele mõjuvad kujujõud oleksid nullid.