An Integral Representation Result for Continuum Γ-Limits of Atomistic Systems in Elasticity Theory

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Abstract

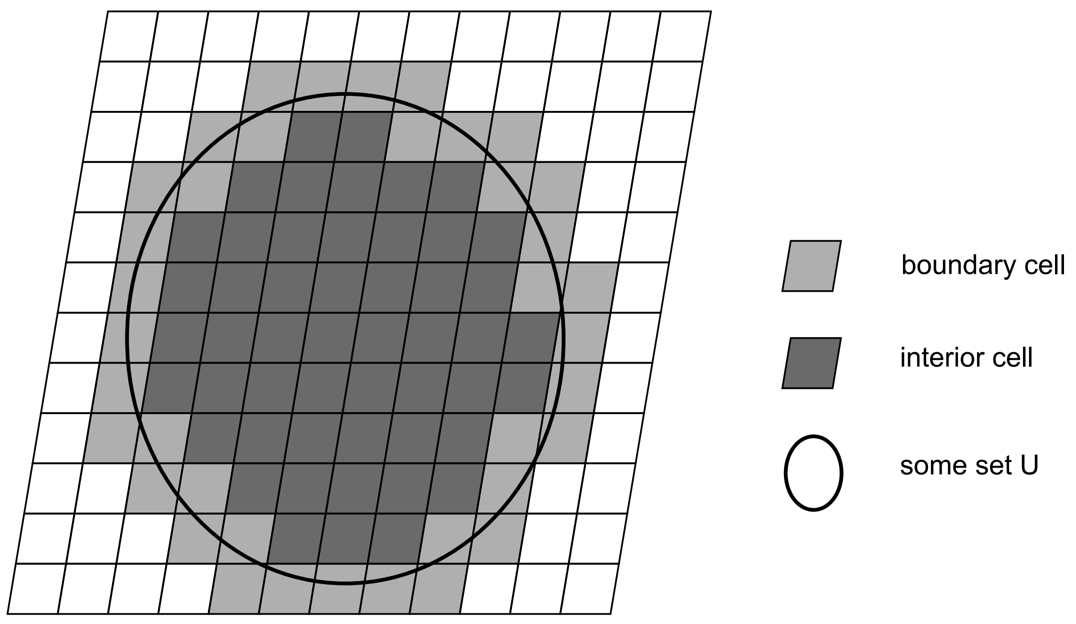
In this thesis we derive continuum limits of atomistic models in the realm of nonlinear elasticity theory rigorously as the interatomic distance tends to zero. In more detail, we obtain as a Γ-limit in the continuum theory an integral functional acting on the deformation gradient, which depends on the underlying atomistic interaction potentials and the lattice geometry. The interaction potentials to which our theory applies are general finite range potentials, which in particular can also account for multi-pole interactions and bond-angle dependent contributions.

Introduction

The main aim of this thesis is to provide a rigorous derivation of nonlinear elasticity functionals from atomistic models. A fundamental contribution towards this aim has been made by Alicandro and Cicalese in (1), where they prove a general integral representation result for continuum limits of atomistic interaction potentials. It is our main aim, departing from this result, to derive a continuum theory for more general interaction potentials which are not restricted to pure pair potentials using some techniques developed by Schmidt in (2).
Furthermore, we rigorously discuss the applicability of the classical ansatz to get a continuous limit, namely, the Cauchy-Born rule. Roughly, the Cauchy-Born rule states that local microscopic deformations follow the macroscopic deformation gradient.

The discrete model

Let U be the 'macroscopic' domain occupied by the elastic body and $\mathcal{L}$ some lattice of the form $\mathcal{L} = A\mathbb{Z}^d$, $A \in \mathbb{R}^{d\times d}$, $\det(A) \neq 0$. Furthermore, let $\varepsilon > 0$ be some small parameter, which scales the interatomistic distances. We define the scaled lattices $\mathcal{L}_\varepsilon = \varepsilon\mathcal{L}$. The scaled lattice $\mathcal{L}_\varepsilon$ divides U into interior and boundary cells as shown in the picture below.



If we call the values of a deformation on the corners of a cell $y_1, \dots, y_{2^d}$ and if we call their arithmetic mean $\bar{y}$, then we can define the discrete gradient as

$$\bar{\nabla} y = \varepsilon^{-1}(y_1 - \bar{y}, \dots, y_{2^d} - \bar{y}).$$

We define our discrete energy by

$$F_\varepsilon(y,U) = \begin{cases} \varepsilon^d \sum\limits_{\text{int-cells}(U)} W_{cell}(\bar{\nabla} y) & \text{if } y \text{ is constant on every cell,} \\ \infty & \text{else.} \end{cases},$$

where the sum takes into account all interior cells with respect to U. The factor ε^d ensures that we have the units energy per volume.

The main result

We can now state our main result. To simplify notations, we define the sets $P_h = A(0,h)^d$.

Theorem. *Suppose that W_{cell} has p-growth. Then, in the limit $\varepsilon \to 0$, $F_\varepsilon(\cdot,\Omega)$ $\Gamma(L^p(\Omega;\mathbb{R}^d))$-converges to the functional F, defined by*

$$F(y) = \begin{cases} \int_\Omega f_{cont}(\nabla y(x))\,dx & \text{if } y \in W^{1,p}(\Omega;\mathbb{R}^d), \\ \infty & \text{otherwise.} \end{cases}$$

Here $f_{cont}\colon \mathbb{R}^{d\times d} \to [0,\infty)$ is given by

$$f_{cont}(M) = \frac{1}{|P_1|}\lim_{N\to\infty}\frac{1}{N^d}\inf\Big\{ \sum_{\text{int-cells}(P_h)} W_{cell}(\bar{\nabla} y) \colon y \text{ constant on every cell and } y(x) = Mx \text{ at corners of boundary cells}\Big\}.$$

Sketch of the proof

The proof is divided into four important steps.

(i) Compactness. We find a subsequence and a functional $F = F(y,U)$ such that all the functionals $F_{\varepsilon_k}(\cdot,U)$, for $U \subset \Omega$ open, Γ-converge to some $F(\cdot,U)$.

(ii) Integral representation. We check that F satisfies the assumptions of a general representation result for functionals on Sobolev spaces. This requires a lot of technical lemmata about the discrete deformations. As a main tool, we use a specific continuous, piecewise affine interpolation of the discrete deformations which was used by Schmidt in (2).

(iii) The boundary value problem. We show that the Γ-convergence result still holds true, if we impose boundary conditions on the boundary cells in the discrete setting and on the boundary in the continuum setting. We prove the convergence of minimizers.

(iv) Homogenization. Using the quasiconvexity of the limit density function and the convergence of minimizers, we show that in fact the limit density function is given by a homogenization formula as stated in the theorem. But this means, that the limit functional is unique. Hence the compactness result is actually a convergence result.

The Cauchy-Born rule

The Cauchy-Born rule states, that if we impose affine boundary conditions, the minimizer of the elastic energy is given exactly by this affine map. That this is indeed true for deformations near to $SO(d)$ under certain assumptions is shown for example in (3) by Conti, Dolzmann, Kirchheim and Müller. This helps us to find a much easier representation for f_{cont}.
Let Z be the discrete gradient of the identity.

Theorem. *Additionally to the assumptions in our main theorem, let the following assumptions be true:*

1. *We have $p \geq d$, $W_{cell} \geq 0$ and $W_{cell}(A) = 0$ if and only if $A = RZ + (c,\dots,c)$.*
2. *W_{cell} is invariant under translations and rotations.*
3. *W_{cell} is smooth in a neighborhood of $SO(d)Z$ and $D^2W_{cell}(Z)$ is positive definite on the orthogonal complement of the subspace spanned by translations and infinitesimal rotations.*

Then there is a neighborhood $\mathcal{U}$ of SO(d), such that

$$f_{cont}(M) = \frac{1}{|\det(A)|}W_{cell}(MZ)$$

for every $M \in \mathcal{U}$.

References

(1) Alicandro, R. , Cicalese, M.: A General Integral Representation Result for Continuum Limits of Discrete Energies with Superlinear Growth, SIAM J. Math. Anal. 36(1):1-37(2004).

(2) Schmidt, B.: On the derivation of linear elasticity from atomistic models, Networks and Heterogeneous Media 4(4):789-812(2009).

(3) Conti, S., Dolzmann, G., Kirchheim, B. and Müller, S.: Sufficient conditions for the validity of the Cauchy-Born rule close to $SO(n)$, J. Eur. Math. Soc. (JEMS) 8:515-539(2006).