Mathematical derivation of a rubber-like stored energy functional

Roberto Alicandro [a], Marco Cicalese [b], Antoine Gloria [c]

[a] DAEIMI, Università di Cassino, via Di Biasio 43, 03043 Cassino (FR), Italy
[b] Dipartimento di Matematica e Applicazioni 'R. Caccioppoli', Università di Napoli, via Cintia, 80126 Napoli, Italy
[c] CERMICS - ENPC, 6 et 8 avenue Blaise Pascal - Champs sur Marne, 77455 Marne la Vallée Cedex 2, France

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Abstract

In this note, we consider a stochastic network of interacting points to which we associate an energy. We study the variational convergence of such an energy when the typical distance of the network goes to zero. We prove that the limit energy can be written as an integral functional, whose energy density is deterministic, hyperelastic and frame-invariant. This derivation allows us in particular to obtain a continuous energy density associated to cross-linked polymer networks. *To cite this article: A. Name1, A. Name2, C. R. Acad. Sci. Paris, Ser. I 340 (2005).*

Résumé

Dérivation mathématique d'une densité d'énergie hyperélastique pour des polymères réticulés. Dans cette note, nous considérons un réseau stochastique de points en interaction auquel nous associons une énergie. Nous étudions alors la convergence variationnelle de cette énergie lorsque la distance caractéristique du réseau tend vers zéro. Nous démontrons que l'énergie limite s'écrit comme l'intégrale d'une densité d'énergie déterministe, hyperélastique et objective. Cette dérivation couvre en particulier des modèles de réseau de polymères réticulés. *Pour citer cet article : A. Name1, A. Name2, C. R. Acad. Sci. Paris, Ser. I 340 (2005).*

1. Introduction

As a starting point, we consider a particular case of the stochastic networks introduced by Blanc, Le Bris and Lions in [4,3]. In what follows, $(\Omega, \mathcal{F}, P)$ denotes a given probability space. Let $\Lambda = \{x_i\}_{i\in\mathbb{Z}^d} \in \left(\mathbb{R}^d\right)^{\mathbb{Z}^d}$ be a set of points. We say that Λ is an admissible set of points if it satisfies the three following conditions:

Email addresses: alicandr@unicas.it (Roberto Alicandro), cicalese@unina.it (Marco Cicalese), gloria@cermics.enpc.fr (Antoine Gloria).

i. there exists $R > 0$ such that $\#\Lambda \cap B(x, R) > 0$ for all $x \in \mathbb{R}^d$;
ii. there exist $R' > 0$ and $k \in \mathbb{N}$ such that $\#\Lambda \cap B(x, R') \leq k$ for all $x \in \mathbb{R}^d$;
iii. there exists $r > 0$ such that $d(x_i, \Lambda \setminus \{x_i\}) \geq r$ for all $i \in \mathbb{Z}^d$.

In particular, to each admissible set of points Λ one can associate a Delaunay triangulation $\mathcal{D}(\Lambda)$.

A stochastic lattice $\mathcal{L} : \Omega \to \left(\mathbb{R}^d\right)^{\mathbb{Z}^d}$ is said to be admissible, if for P-almost every $\omega \in \Omega$, $\mathcal{L}(\omega)$ is an admissible set of points, and if the Delaunay triangulation is regular in the sense of the interpolation theory. Given a measure preserving group $\{\tau_{\mathbf{k}}\}_{\mathbf{k}\in\mathbb{Z}^d}$ acting on Ω, $\mathcal{L}$ is said to be stationary if $\mathcal{L}(\tau_{\mathbf{k}}(\omega)) = \mathcal{L}(\omega) - \mathbf{k}$ for all $\mathbf{k} \in \mathbb{Z}^d$ and ergodic if, for any $A \in \mathcal{F}$, $\tau_{\mathbf{k}}(A) = A$ implies $P(A) = 0$ or $P(A) = 1$. Note that in two dimensions, any admissible set of points has a regular Delaunay triangulation. In three dimensions, the conditions *i.*, *ii.* and *iii.* are not sufficient to ensure the existence of a regular triangulation.

To each realization ω of the stochastic lattice, we associate an energy which only depends on the realization. For all regular bounded open subset A of $\mathbb{R}^d$, and all $u : \mathcal{L}(\omega) \to \mathbb{R}^n$, we define the energy of the lattice by

$$E(u, A)(\omega) = \sum_{x_i \in \mathcal{L}(\omega)\cap A} \sum_{\substack{x_j \neq x_i \in \mathcal{L}(\omega) \cap A \\ [x_i, x_j] \subset A}} J(x_j - x_i) f\left(\frac{u(x_j) - u(x_i)}{|x_j - x_i|}\right), \tag{1}$$

where $J : \mathbb{R}^d \to \mathbb{R}$ and $f : \mathbb{R}^n \to \mathbb{R}$ are given functions that do not depend on ω and A and where $[x_i, x_j] = tx_i + (1-t)x_j$, $t \in [0, 1]$. The precise forms of J and f will be prescribed in the following section.

In what follows we consider a scaled version of the energy in (1); i.e. for all $\varepsilon > 0$, and $u_\varepsilon : \varepsilon\mathcal{L}(\omega) \to \mathbb{R}^n$, we set

$$E_\varepsilon(u_\varepsilon, A)(\omega) = \sum_{x_i \in \varepsilon\mathcal{L}(\omega)\cap A} \varepsilon^d \sum_{\substack{x_j \neq x_i \in \varepsilon\mathcal{L}(\omega) \cap A \\ [x_i, x_j] \subset A}} J\left(\frac{x_j - x_i}{\varepsilon}\right) f\left(\frac{u_\varepsilon(x_j) - u_\varepsilon(x_i)}{|x_j - x_i|}\right). \tag{2}$$

2. Derivation of a macroscopic model

2.1. *Main result*

We make the following set of assumptions (H) on the energy E_ε:

$$(H) \qquad \begin{cases} \text{There exist } p > 1, C_1, C_2 > 0, \text{ such that } C_1|v|^p - 1 \leq f(v) \leq C_2|v|^p + 1, \quad \forall v \in \mathbb{R}^n \\ J \geq 0 \text{ and } \inf\limits_{B(0,4R)} J(z) > 0 \\ \int\limits_{\mathbb{R}^d} J(z)dz < \infty \end{cases}$$

In particular, if $n = d$ and for all $w \in S^1(\mathbb{R}^d)$, $f(w) = 0$, then $u : x \mapsto x$ is a minimizer of the discrete energy and the lattice is a ground state of the system of interacting points. This may model in particular the ground state of a rubber-like polymer at the scale of the polymer chain (see [11]).

For all $\omega \in \Omega$, let $\mathcal{T} = \{T_i\}_{i\in\mathbb{Z}^d}$ be the set of the triangles of a regular Delaunay triangulation associated to $\varepsilon\mathcal{L}(\omega)$. In what follows, in order to study the asymptotics of the energy in (2) as $\varepsilon \to 0$ in the framework of Γ-convergence (see [5] for an introduction to the subject), we identify each $u : \varepsilon\mathcal{L}(\omega) \to \mathbb{R}^n$ with its continuous piecewise affine interpolation on $\mathcal{T}$.

Theorem 1 *Let D be an open bounded subset of $\mathbb{R}^d$, $\mathcal{L} : \Omega \to \left(\mathbb{R}^d\right)^{\mathbb{Z}^d}$ be an admissible stationary and ergodic stochastic lattice, and let f and J satisfy Hypotheses (H). For P-almost all $\omega \in \Omega$, $E_\varepsilon(\cdot, D)(\omega)$ $\Gamma - L^p(D)$ converges to $E(\cdot, D)$ which is finite on $W^{1,p}(D)$ and defined by*

$$E(v, D) = \int_D W_{hom}(\nabla v(x))dx, \tag{3}$$

where W_{hom} is an homogeneous in space quasiconvex energy density satisfying a growth condition of order p, and given by the following asymptotic formula

$$\begin{aligned} W_{hom}(\xi) = \lim_{N\to\infty} \frac{1}{N^d} \int_\Omega \inf \big\{ & E_1(u, (0, N)^d)(\omega), u(z) = \xi \cdot z \text{ for } z \in \mathcal{L}(\omega), \\ & dist(z, \partial(0, N)^d) \leq 2R \big\}\, dP(\omega), \end{aligned} \tag{4}$$

In addition, infimum problems with prescribed boundary conditions also converge.

2.2. *Sketch of the proof*

The details of the following proof will be given in [2].

Individual compactness. The first step of the proof consists in obtaining individual compactness. For all $\omega \in \Omega$, we prove that there exists a subsequence ε_n, such that $E_{\varepsilon_n}(\cdot, D)(\omega)$ Γ-converges to some $E(\cdot, D)(\omega)$ on $W^{1,p}(D)$, for any open bounded regular subset $D \subset \mathbb{R}^d$. To this end, one proceeds as in [1]. The estimates are however more delicate to get. Fixed a regular Delaunay triangulation associated to ω, one first singles out the contribution to the energy due to the interactions between nearest-neighbors, by which we mean two vertices of the same triangle, and, using the coercivity hypothesis on f, obtain the coercivity of the Γ-liminf. Up to introducing a coarser periodic reference lattice, one can classify the interactions according to their range. This allows us to adapt the argument used in [1] where the periodic-lattice case is considered in the deterministic setting and to get the growth condition from above and the measure property as set function of the Γ-limsup $E_\varepsilon(u, A)$ for any regular open set $A \subset \mathbb{R}^d$. Using then the compactness property of Γ-convergence and the integral representation result in [6], we prove that, up to extractions, there exists a Γ-limit $E(\cdot, D)(\omega)$, which can be expressed in terms of an integral functional. The second part of the proof is devoted to show that $E(\cdot, D)(\omega)$ does not depend on ω and that the associated energy density W_{hom} does not depend on the space variable.

Ergodicity of subadditive processes. The result is achieved if we prove the existence of the limit (4) for the asymptotic formula. The proof relies on the subadditive ergodic theorem, and more precisely on the variant used in [8]. The energy $E_1(\cdot, D)$ is not subadditive since the interactions are not local. So is its infimum. One may however introduce a modified energy defined on the borelians of $\mathbb{R}^d$, which is subadditive and such that the asymptotic limits of type (4) coincide for both energies, the convergence of one implying the convergence of the other. Doing so, the ergodic theorem shows the existence of (4) and therefore concludes the proof. Let us quickly define the modified energy in the case of finite-range interactions, namely $\exists L \in \mathbb{N} : \ J(z) = 0$ if $|z| > L$. Let $B \in \mathcal{B}(\mathbb{R}^d)$ be a bounded borelian set. We denote by $\overline{C}(B)$ the union of the finite number of closed unit cubes C centered in points of $\mathbb{Z}^d$ such that $C \cap B \neq \emptyset$, and by $C(B)$ the interior of $\overline{C}(B)$. For all $\alpha > 0$ and for all $\xi \in \mathcal{M}_d(\mathbb{R})$, we set

$$G^\xi(B)(\omega) = \inf\{E(u, C(B))(\omega), u(x_i) = \xi \cdot x \text{ if } \mathrm{d}(x_i, \partial C(B)) \leq R\} + \alpha \operatorname{perim}(C(B)),$$

where perim denotes the perimeter of the set. For all ξ, there exists α big enough such that G^ξ is a subadditive set functional. In addition, for regular sets B, $\lim_{|t|\to\infty} \frac{1}{|tB|} \alpha \operatorname{perim}(C(tB)) = 0$. Therefore, [8, Prop. 1] implies the existence of $\lim_{|t|\to\infty} \frac{1}{|tB|} G^\xi(tB)(\omega)$ and its independence upon ω, which concludes the proof.

3. Remarks and extensions

Some comments are in order. First, it is easily shown that W_{hom} is frame-invariant. Second, if there exists a stationary action group of rotations, then W_{hom} is isotropic.

Volume effects are not taken into account in Theorem 1. Given a regular Delaunay triangulation associated to the lattice, one can slightly modify the energy of the lattice by adding a term penalizing volume changes on each triangle of $\mathcal{T}$ and satisfying a growth condition of order p from above. In such a case, Theorem 1 also holds. However, this modification does not cover incompressible behaviours and does not preserve the orientation. To obtain more realistic energy densities, one may proceed in two steps: first use a cut-off η on the 'realistic' volumetric energy (see [7]) in order to make it satisfy a suitable growth condition and pass to the limit as $\varepsilon \to 0$, and then let the cut-off parameter η go to infinity to recover the 'original' volumetric properties. However it is not clear whether it is possible to switch the limits. These remarks and extensions will be detailed in a forthcoming paper [2].

We finally point out that the variational convergence of stochastic energies defined on a one-dimensional periodic network of points in interaction has been considered in [9,10].

References

[1] R. Alicandro and M. Cicalese. A general integral representation result for the continuum limits of discrete energies with superlinear growth. *SIAM J. Math. Anal.*, 36(1):1–37, 2004.

[2] R. Alicandro, M. Cicalese, and A. Gloria. Integral representation results for energies defined on stochastic lattices and application to nonlinear elasticity, *in preparation*.

[3] X. Blanc, C. Le Bris, and P.L. Lions. Du discret au continu pour des réseaux aléatoires d'atomes. *C. R. Acad. Sci. Paris, Série I*, 342:627–633, 2006.

[4] X. Blanc, C. Le Bris, and P.L. Lions. The energy of some microscopic stochastic lattices. *Arch. Rational Mech. Anal.*, to appear.

[5] A. Braides Γ-*convergence for beginners,* volume 22 of *Oxford Lecture Series in Mathematics and its Applications.* Oxford University Press, 2002.

[6] G. Buttazzo and G. Dal Maso. Integral representation and relaxation of local functionals. *Nonlinear Anal.*, 9(6):515–532, 1985.

[7] P.G. Ciarlet. *Mathematical elasticity. Vol. I*, volume 20 of *Studies in Mathematics and its Applications.* North-Holland Publishing Co., Amsterdam, 1988.

[8] G. Dal Maso and L. Modica. Nonlinear stochastic homogenization and ergodic theory. *J. Reine Angew. Math.*, 368:28–42, 1986.

[9] O. Iosifescu, C. Licht, and G. Michaille. Variational limit of a one-dimensional discrete and statistically homogeneous system of material points. *C. R. Math. Acad. Sci. Paris*, 32:575–580, 2001.

[10] O. Iosifescu, C. Licht, and G. Michaille. Variational limit of a one-dimensional discrete and statistically homogeneous system of material points. *Asymptot. Anal.*, 28:309–329, 2001.

[11] L.R.G. Treolar *The physics of rubber elasticity.* Oxford at Clarendon Press, Oxford, 1949.