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Material Theories

Organised by
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Abstract. Material theories is a series of workshops concerned with a broad range of topics related to the mechanics and mathematics of materials. As such, this edition brought together researchers from diverse fields converging toward the interaction between mathematics, mechanics, and material science.

Mathematics Subject Classification (2010): 70-xx, 74-xx, 76-xx, 82-xx.

Introduction by the Organisers

The workshops focusing on Material Theories take place in Oberwolfach for more than 30 years. This year workshop was organized by Sergio Conti (Bonn), Antonio DeSimone (Trieste), Stephan Luckhaus (Leipzig), and Lev Truskinovsky (Paris). It was well attended with over 50 participants covering a broad geographic area.

The goal of this series of workshops is to bring together mechanicians, physicists and mathematicians and to expose in this way the applied mathematics community to new and exciting developments in the fields of material science, statistical physics and even biology. At the 2017 workshop the main emphasis was placed on contributions attempting to bridge the gap between discrete and continuum approaches, focusing on the multi-scale nature of physical phenomena, and most importantly requiring new and nontrivial mathematics. The workshop created new possibilities for the synergistic interaction between different disciplines which should potentially lead to new progress in the understanding of material behavior.

The range of topics at the workshop was very broad, from the new ways of selecting weak solutions of Euler equations (Brenier), stochastic homogenization

of random composites (Otto, Zeppieri) and exact results in the theory of nonequilibrium steady states (Redig) to the study of the relation between quasi-convexity and rank one convexity (Grabovsky) and new approaches to solitons in lattices (Vainchtein). A particular focus was on the description of plastic behavior of crystalline and amorphous materials at the mesoscopic scale accounting for marginal stability and criticality (Wyart, Lerner). A series of talks was devoted to shells and plates, including those with embedded incompatibility (Agostiniani, Lewicka, Sharon) and to rigorous results in the description of distributed dislocations by non Riemanian geometry with torsion (Kupferman). Dislocational structures were also discussed in the context of energy minimization in nonconvex variational problems (Garroni, Scardia). New mathematical problems in fracture mechanics were discussed as well (Chambolle, Francfort). Other subjects included cloacking (Yavari), trapping of elastic waves by obstacles (Smyshlyaev), topological defects in liquid crystals (Kamien), crystallization and the Cauchy-Born rule (Alberti, Schmidt, Stefanelli). Considerable attention was given to the problems of biomechanics and mechanics of active matter including the talks on growth induced buckling during development (Ciarletta), cell motility (Giomi, Preziosi) and active rheology (Clement). The format of the workshop has again proved to be very successful, furnishing new problems to the applied mathematics community and building new interdisciplinary collaborations.

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Workshop: Material Theories

Table of Contents

Abstracts

Heterogeneous elastic plates with lateral modulation of the *target* curvature

Virginia Agostiniani
(joint work with A. Lucantonio, D. Lučić)

Inspired by the modelling of nematic elastomer ribbons and of thin gel sheets, we consider a general framework which accounts for thin sheets of a material characterised by heterogeneous spontaneous stretches. In the 3D mathematical description, these spontaneous stretches are the minimisers of a (heterogeneous) energy density, are a perturbation of order h (= the small thickness thickness parameter) of the identity, and depend on both the planar and the thickness variables. The corresponding 2D Kirchhoff model, which is constrained to the set of isometric immersions of the mid-plane into $\mathbb{R}^3$, penalises deviations of the second fundamental form associated with a deformation from a target curvature tensor. We then characterise isometries which minimise the 2D energy functional by minimising the integrand pointwise, in the case when the target curvature is piecewise constant.

The initial value problem for the Euler equations of incompressible fluids viewed as a concave maximization problem of optimal transport type

Yann Brenier

Solving initial value problems by convex minimization techniques is definitely not a new idea, in particular in the framework of linear evolution PDEs, as illustrated by the classical least square method. For instance, in the case of a linear transport equation such as $\partial_t u + \partial_x u = 0$, one can try to minimize

$$\int\int (\partial_t u + \partial_x u)^2 dxdt, \quad u(0,\cdot) = u_0,$$

where u_0 is the initial condition. This typically leads to (degenerate) space-time elliptic problems. In the framework of nonlinear equation, similar strategies can be used but usually lead to non-convex ill-conditioned minimization problems. In this abstract, we discuss a somewhat different strategy for the class of systems of conservation laws with a strictly convex entropy [4], namely

$$\partial_t U + \partial_i(F^i(U)) = 0, \;\; \partial_t E(U) + \partial_i Q^i(U) = 0,$$

where $U = U(t,x) \in \mathbb{R}^m$, $x \in \mathcal{D} \subset \mathbb{R}^d$, $t \in [0,T]$, F, E, Q, being respectively the flux, entropy and entropy-flux functions, with appropriate boundary conditions (for simplicity, we restrict ourself to the periodic case, when $\mathcal{D} = (\mathbb{R}/\mathbb{Z})^d$). This class contains many classical models in continuum mechanics and material sciences (Euler equations of hydrodynamics, Elastodynamics with polyconvex energy, ideal

Magnetohydrodynamics, etc...[4]). In our talk, we have focused on the borderline case of the Euler equations of incompressible inviscid fluids for which rigorous results have been recently established [3], but we will expose here the strategy for the more general framework of conservation laws with convex entropy. Let us start with the min-max problem

$$I = \inf_U \sup_W \int_0^T \int_{\mathcal{D}} E(U) - \partial_t W_\alpha U^\alpha - \partial_i W_\alpha F^{\alpha i}(U)\, dxdt - \int_{\mathcal{D}} W_\alpha(0,x) U_0^\alpha(x) dx,$$

where $W = W(t,x) \in \mathbb{R}^m$ are smooth test functions, vanishing at $t = T$. This amounts to look for a weak solution U of our system of conservation laws with initial condition U_0 that minimizes the time integral of its entropy. A priori, this sounds silly since we already assume U to be a solution and we know (at least for smooth solutions) that the entropy is conserved in time, depending only on the initial condition U_0, so that there is a priori nothing to minimize. However, for a fixed initial condition, weak solutions may not be unique and the conservation of entropy is generally not true. (This is now well established in the case of the Euler equations, in Hydrodynamics, through the results of Scheffer, Shnirelman, De Lellis-Székelyhidi Jr. [7, 8, 5, 10].) Concerning the min-max problem, let us now exchange the infimum and the supremum in the definition of I and get the lower bound

$$J = \sup_W \inf_U \int_0^T \int_{\mathcal{D}} E(U) - \partial_t W \cdot U - DW : F(U)\, dxdt - \int_{\mathcal{D}} W(0,\cdot) \cdot U_0\, dx$$

(with obvious abridged notations), which can be reduced to

$$J = \sup_W \int_0^T \int_{\mathcal{D}} -K(\partial_t W, DW) dxdt - \int_{\mathcal{D}} W(0,\cdot) \cdot U_0\, dx,$$

where W is still subject to $W(T,\cdot) = 0$ and K is the *convex* function defined by

$$K(A,B) = \sup_{U \in \mathbb{R}^m} A_\alpha U^\alpha + B_{\alpha i} F^{\alpha i}(U) - E(U), \quad A \in \mathbb{R}^m, \quad B \in \mathbb{R}^{m \times d}.$$

This concave maximization problem is very similar to the Monge optimal mass transport problem with quadratic cost in its so-called "Benamou-Brenier" formulation [2, 1, 9]. Its numerical treatment in the style of [2] is currently under investigation. The simplest example of such a maximization problem is provided by the (so-called) inviscid Burgers equation:

$$\partial_t U + \partial_x(\frac{U^2}{2}) = 0, \quad U = U(t,x) \in \mathbb{R}, \quad x \in \mathbb{R}/\mathbb{Z}, \quad t \in [0,T],$$

where it reads

$$J = \sup_W \int_0^T \int_{\mathcal{D}} -\frac{\partial_t W^2}{2(1-\partial_x W)} dxdt - \int_{\mathcal{D}} W(0,\cdot) \cdot U_0\, dx,$$

with $W = W(t,x) \in \mathbb{R}$ subject to $\partial_x W \leq 1$ and $W(T,\cdot) = 0$.
In [3], we have studied the (borderline) case of the Euler equations of incompressible fluids

$$\partial_t U + \nabla \cdot (U \otimes U) + \nabla p = 0, \quad \nabla \cdot U = 0, \quad U = U(t,x) \in \mathbb{R}^d, \quad p = p(t,x) \in \mathbb{R}.$$

Then, the maximization problem reads:

$$\sup_{A, \nabla \phi} \; -\int_0^T \int_{\mathcal{D}} (\partial_t A + \nabla \phi) \cdot \frac{(\mathbb{I}_d - \nabla A - \nabla A^T)^{-1}}{2} \cdot (\partial_t A + \nabla \phi) dx dt - \int_{\mathcal{D}} A(0,\cdot) \cdot U_0 \, dx$$

where $A = A(t,x) \in \mathbb{R}^d$ is a divergence-free vector field that vanishes at $t = T$, while ϕ is an additional scalar field needed to enforce the incompressibility condition. We have obtained the following results [3]:
i) for all initial data $U_0 \in L^2$, there is always an optimal solution A with $\partial_t A \in L^2$ and $\nabla A + \nabla A^T \in L^\infty$;
ii) any smooth solution of the Euler equations $U(t,x)$ can be recovered for short enough times (more precisely, as long as

$$(T-t)^{-1} \mathbb{I}_d + (\nabla U + \nabla U^T)(t,x) \tag{1}$$

stays positive, as a symmetric matrix, for all $x \in \mathcal{D}$ and $t \in [0,T]$, which is reminiscent of the Ponce regularity criterium for the Euler equations -see [6]).
In addition, the maximization problem can be related to the theory of sub-solutions to the Euler equations which has recently attracted a lot of interest after the celebrated work of De Lellis and Székelyhidi [5] in the framework of Convex Integration theory.

References

[1] L. Ambrosio, N. Gigli, G. Savaré, *Gradient flows in metric spaces and in the space of probability measures,* Lectures in Mathematics ETH Zürich, Birkhäuser , 2008.
[2] J.-D. Benamou, Y. Brenier, *A Computational Fluid Mechanics solution to the Monge-Kantorovich mass transfer problem,* Numer. Math. 84 (2000) 375-393.
[3] Y. Brenier, *The initial value problem for the Euler equations of incompressible fluids viewed as a concave maximization problem ,* arXiv:1706.04180.
[4] C. Dafermos, *Hyperbolic conservation laws in continuum physics,* Springer, 2000.
[5] C. De Lellis, L. Székelyhidi, László, Jr. *The Euler equations as a differential inclusion,* Ann. of Math. (2) 170 (2009) 1417-1436.
[6] P.-L. Lions, *Mathematical topics in fluid mechanics. Vol. 1. Incompressible models,* Oxford 1996.
[7] V. Scheffer, *An inviscid flow with compact support in space-time,* J. Geom. Anal. 3 (1993) 343-401.
[8] A. Shnirelman, *On the nonuniqueness of weak solution of the Euler equation,* Comm. Pure Appl. Math., 50 (1997) 1261-1286,
[9] C. Villani, *Topics in Optimal Transportation,* Grad. Stud. Math., vol. 58, AMS 2003.
[10] E. Wiedemann *Existence of weak solutions for the incompressible Euler equations,* Ann. Inst. H. Poincaré Anal. Non Linéaire, 28 (2011) 727-730...

Phase-field approximations of Griffith energies and crack non-interpenetration

Antonin Chambolle
(joint work with S. Conti, G. Francfort)

The variational approach to fracture [12, 5] is an extension of Griffith's classical theory for the modelling and study of crack growth, where, in a quasistatic setting, a crack evolution is computed by successive (global) minimisations of an energy consisting of a "bulk" (linearised elasticity) part and a "crack" term which penalises the length or surface of the discontinuity of the displacement. Namely, given a boundary datum U_0 on a part of $\Gamma^D \subseteq \partial\Omega$, $\Omega \in \mathbb{R}^d$ ($d = 2, 3$ in general), and a "time"-step $\delta t > 0$, one finds at each step $k \geq 1$ a minimiser (u, K) of

$$\min\left\{\int_\Omega \mathbb{C}e(u) : e(u)dx + \mathcal{H}^{d-1}(K) : u = (k\delta t)U_0 \text{ on } \Gamma^D, K \supset K^{k-1}\right\}. \tag{1}$$

The tensor $\mathbb{C}$ is the Hooke's law, typically $\mathbb{C}e(u) = 2\mu e(u) + \lambda \mathrm{Tr}\, e(u) Id$ and $e(u) = (Du + Du^T)/2$ is the symmetrised gradient of the displacement, here a function $u \in H^1_{loc}(\Omega \setminus K; \mathbb{R}^d)$.

In practice, one need to relax a bit this problem (for which existence remains unknown, see [14, 9] for recent results) in the class "$[G]SBD$" [1, 4, 11] of functions u such that $Du + Du^T$ is a bounded Radon measure, which is decomposed into a part $e(u)dx$ absolutely continuous with respect to Lebesgue's measure, and a $(d-1)$-dimensional "jump" part $[u] \odot \nu_u \mathcal{H}^{d-1} \llcorner J_u$, where the countably $(d-1)$-rectifiable set J_u is defined as the set of points x where there exists (a normal unit vector) ν_u and (two different displacement values) $u^\pm$ such that, as $\rho \to 0$,

$$y \mapsto u(x + \rho y) \overset{L^1(B_1)}{\longrightarrow} u^+ \chi_{\{y\cdot\nu_u \geq 0\}} + u^- \chi_{\{y\cdot\nu_u < 0\}}$$

(the blowup of u at x converges to a function taking two values). Then, $[u] = u^+ - u^-$ and $[u] \odot \nu_u = ([u] \otimes \nu_u + \nu_u \otimes [u])/2$.

Numerical methods to tackle this problem are typically based on phase-field approximations in the spirit of [2], see [5]. One important issue with this model, is that it is symmetric with respect to a change of sign of the external loading $U_0 \to -U_0$: hence "physical" deformations with opening cracks can easily be turned into "non-physical" experiments where the crack is collapsing into itself, and interpenetrating. Quite a few models have been proposed to solve this issue, see [3, 15, 13, 16], in the framework if phase-field approximations.

Our paper [7] shows, in dimension 2, that the simulations presented in these papers are coherent with a limiting model with non-interpenetration. For instance, consider the most simple linearised non-interpenetration constraint, which requires that $[u]\cdot\nu_u \geq 0$ almost everywhere on the jump (the angle between the opening and the normal to the jump is acute). In terms of the measure $Eu = (Du + Du^T)/2$, it is equivalent to requiring that

$$E^s u = [u] \cdot \nu_u \mathcal{H}^{d-1} \llcorner J_u \geq 0 \tag{2}$$

(the singular part of the measure Eu is nonnegative). In other words, $(\operatorname{div} u)^- \in L^2(\Omega)$.

The adaption of [2] to tackle this model reads [3]:

$$\mathcal{E}_\varepsilon(u,v) = \int_\Omega (\eta_\varepsilon + v^2)(\mathbb{C}e(u) : e(u) - k((\operatorname{div} u)^-)^2) + k((\operatorname{div} u)^-)^2)dx \\ + \int_\Omega \varepsilon|\nabla v|^2 + \frac{(1-v)^2}{4\varepsilon}dx$$

where $k > 0$ is any number such that $\mathbb{C}S : S \geq k(\operatorname{Tr}(S))^2$ for all symmetric tensors S. Here, v is a field which will go to 1 almost everywhere but on the jump of u, as $\varepsilon \to 0$. The parameter $\eta_\varepsilon = o(\varepsilon)$ is just here to make the problem well-posed in H^1 and is not strictly necessary.

For $k = 0$, it is known that $\mathcal{E}_\varepsilon$ (with an additional global L^∞ constraint on the displacements u) Γ-converges to the energy in (1) as $\varepsilon \to 0$ [6].

Our main theorem states that in dimension 2, for $k > 0$, $\mathcal{E}_\varepsilon$ Γ-converges, as $\varepsilon \to 0$, to the same energy plus the additional constraint (2). The "liminf" part of the convergence is clear, as the energy for $k > 0$ is larger than for $k = 0$, and forces $(\operatorname{div} u)^-$ to remain bounded in L^2.

The difficulty is to build a correct recovery sequence. One cannot rely on an approximation result such as in [2, 6], which is far from clear with the constraint (2). Our proof, built upon a result in [8] which shows that SBD fields with small jump set and $e(u) \in L^2$ can be approximated with L^2 functions, consists in building a recovery sequence u_ε by

(i) convolving u with a smoothing kernel ρ_ε ($u_\varepsilon = \rho_\varepsilon * u$) near the "big" parts of the jump J_u (this *obviously* maintains a global L^2 bound on $(\operatorname{div} u_\varepsilon)^-$, if $(\operatorname{div} u)^- \in L^2$);

(ii) appropriately approximate u with a u_ε locally, where the jump set J_u has a low density, using the techniques developed in [8];

(iii) appropriately glue together the two such obtained approximations u_ε.

It is this last point which we cannot really solve, in dimension larger than 2. We do not really solve it in dimension 2 either, the construction being even simpler: In this case, thanks to a result in [10], we observe that at each scale $\varepsilon > 0$, we can replace u (with a control of the energy) by a function u' which has the property that in a "strip" between the two regions corresponding to points (i) and (ii) above, it has *no jump at all*. In that case, the constructions (i) and (ii) provide exactly the *same* approximation u_ε, so that point (iii) is not even required.

References

[1] L. Ambrosio, A. Coscia, & G. Dal Maso, *Fine properties of functions with bounded deformation*, Arch. Rational Mech. Anal. **139**-3 (1997) 201–238.

[2] L. Ambrosio & V.M. Tortorelli, *Approximation of functionals depending on jumps by elliptic functionals via* Γ*-convergence*, Comm. Pure Appl. Math. **43**-8 (1990) 999–1036.

[3] H. Amor, J.J. Marigo & C. Maurini, *Regularized formulation of the variational brittle fracture with unilateral contact: Numerical experiments*, J. Mech, Phys. Solids **57**-8 (2009) 1209–1229.

[4] G. Bellettini, A. Coscia & G. Dal Maso, *Compactness and lower semicontinuity properties in $SBD(\Omega)$*, Mathematische Zeitschrift **228** (1998) 337–351.
[5] B. Bourdin, G.A. Francfort & J.J. Marigo, *The variational approach to fracture*, J. Elasticity **91**-1,2,3 (2008) 5–148.
[6] A. Chambolle, *An approximation result for special functions with bounded variations*, J. Math Pures Appl. **83** (2004) 929–954.
[7] A. Chambolle, S. Conti & G.A. Francfort, *Approximation of a Brittle Fracture Energy with a Constraint of Non-Interpenetration*, preprint 2017.
[8] A. Chambolle, S. Conti & G.A. Francfort, *Korn-Poincaré inequalities for functions with a small jump set*, Indiana Univ. Math. J. **65**-4 (2016)1373–1399.
[9] S. Conti, M. Focardi, and F. Iurlano, *Existence of minimizers for the 2d stationary Griffith fracture model*, C. R. Math. Acad. Sci. Paris, 354 (2016), pp. 1055–1059.
[10] S. Conti, M. Focardi & F. Iurlano, *Integral representation for functionals defined on SBD^p in dimension two*, *Arch. Ration. Mech. Anal.* **223**-3 (2017) 1337–1374.
[11] G. Dal Maso, *Generalised functions of bounded deformation*, J. Eur. Math. Soc. **15**-5 (2013) 1943–1997.
[12] G. A. Francfort and J.-J. Marigo, *Revisiting brittle fracture as an energy minimization problem*, J. Mech. Phys. Solids, 46 (1998), pp. 1319–1342.
[13] F. Freddi and G. Royer-Carfagni, *Regularized variational theories of fracture: a unified approach*, J. Mech. Phys. Solids, 58 (2010), pp. 1154–1174.
[14] M. Friedrich & F. Solombrino, *Quasistatic crack growth in 2d-linearized elasticity*, to appear in Ann. Inst. H. Poincaré Anal. Non Linéaire (2017).
[15] G. Lancioni & G. Royer-Carfagni, *The Variational Approach to Fracture Mechanics. A Practical Application to the French Panthéon in Paris*, J. Elasticity **95**-1,2 (2009) 1–30.
[16] M. Ortiz, *A constitutive theory for the inelastic behavior of concrete*, Mech. Mater. **1**-4 (1985) 67–93.

Patterning through instabilities in soft solids

Pasquale Ciarletta
(joint work with Davide Riccobelli, Matteo Taffetani)

Classical works in engineering sciences almost exclusively analyze the possibility of instability as a predictive tool to be used in order to avoid the onset of material failure in structural applications. A multidisciplinary research community has been recently coalescing, focused on the idea that instabilities may also be used positively to guide the design and fabrication of new materials [1]. This guiding principle has been employed in designing novel elastic structures, where instabilities provide simple mechanisms through which to generate a switchable morphology, with original applications such as self-folding machines, stretchable electronics and smart textiles. Indeed, the recent technical possibility to generate extreme deformations in complex matter opens the way to unexplored instability regimes, associated to non-trivial phenomena. In fact, the combination of both geometrical and material nonlinearities can prompt the occurrence of intricate morphological changes after multiple bifurcations, often leading to unconventional (or, even, counter-intuitive) behaviors.

This talk is centered on the physical understanding of two classes of instabilities in soft elastic solids.

The first system model proves the possibility to fabricate morphable miniaturized,

very soft elastic filaments, in which the capillary forces are of the same order of the bulk elastic stresses. Whilst the surface tension in a thin fluid filament triggers the formation of droplets, which spontaneously break down, a soft elastic cylinder is always stable if subjected to a homogenous uniaxial extension. The capillary break-down can be therefore stabilized by the elastic effects in a very soft gel with a sufficiently small radius, thus creating either a beaded or a pearled pattern [2]. The pattern formation is provoked by a phase transformation due to the loss of convexity of the total energy induced by capillary effects. In summary, it is possible to tune the filament morphology by simply controlling either the applied axial strain or the capillary tension in a well-identified range [3].
The second system model concerns the shape transition in soft solids due to the effect of gravity. Considering a body composed by two heavy elastic layers, attached to a rigid surface and only subjected to the bulk gravity force, the selection of different patterns as well as their nonlinear evolution is well characterized, unveiling the interplay between elastic and geometric effects for their formation. Unlike similar gravity-induced shape transitions in fluids, as the Rayleigh Taylor instability, the nonlinear elastic effects are proved to saturate the dynamic instability of the bifurcated solutions, displaying a rich morphological diagram where both digitations and stable wrinkling can emerge [4].
In both cases, it is shown that, like in biological materials, the robustness of the morphological control can be enforced by the redundancy of its actuating mechanisms.

References

[1] P. Ciarletta, and D. Vella. *Patterning through instabilities in complex media: theory and applications*, Phil. Trans. R. Soc. A **375** (2017), 20160442.
[2] M. Taffetani, and P. Ciarletta, *Elastocapillarity can control the formation and the morphology of beads-on-string structures in solid fibers*, Physical Review E **91**(3) (2015), p.032413.
[3] M. Taffetani, and P. Ciarletta, *Beading instability in soft cylindrical gels with capillary energy: Weakly non-linear analysis and numerical simulations*, Journal of the Mechanics and Physics of Solids **81** (2015), 91–120.
[4] D. Riccobelli, and P. Ciarletta. *Rayleigh–Taylor instability in soft elastic layers*, Phil. Trans. R. Soc. A **375**, (2017): p.20160421.

Active bacterial fluids : from individual effort to team work

Eric Clement
(joint work with Anke Lindner, Carine Douarche, Harold Auradou)

Bacteria swimming in a fluid induce very deep changes in the macroscopic transport properties and in the constitutive relations of the suspension. We are interested in understanding the hydrodynamics of those bacterial fluids. We currently study various phenomena associated with the swimming activity such as the activated Brownian motion, the emergence of collective motion, the viscous response and the hydrodynamic dispersion. We will discuss how a sheared suspension of bacteria may display a viscosity decreasing with concentration and how at large

concentration, it undergoes a transition to a "superfluid" regime of zero macroscopic viscosity.

References

[1] E. Clement, A. Lindner, C.Douarche, and H. Auradou, Bacterial suspensions under flow, Eur. Phys. J. Special Topics **225**, 2389–2406 (2016).
[2] J. Gachelin,A. Rousselet, A. Lindner & E. Clement, Collective motion in E. coli bacteria suspensions, New Journal of Physics, **16**, 025003 (2014).
[3] H.M.Lopez , J. Gachelin, C. Douarche, H.Auradou, E. Clement, Turning bacteria suspensions into a "superfluid" Phys. Rev. Lett. **115**, 028301 (2015).

Fracture with healing: a toy model for cavitation?

Gilles A. Francfort
(joint work with A. Giacomini, O. Lopez-Pamies)

In the footstep of A.N. Gent & P.B. Lindley [3], cavitation in rubber was viewed for a long time as a purely elastic phenomenon. In essence incipient point defects would expand into spherical cavities under deformations of the form $x/|x|$. This was recast in the mathematical universe by J.M. Ball [1]and his contribution was followed by a great number of promising mathematical studies.

Yet it had already been remarked early on, most notably by M.L. Williams & R.A. Schapery [8] that doing so resulted in unrealistically high elastic strains along the boundary of the cavity. They had suggested that one should complement the Gent-Lindley picture by accounting for possible breakage of the crosslinks, hence introducing a modicum of fracture into the model. This was largely ignored by the "rubber" community until it was picked up by O. Lopez-Pamies at the modeling level and by K. Ravi-Chandar on the experimental end; see e.g. [5].

Actually the resulting picture, which does show a better fit with data, has to be somewhat amended because of the apparent presence of a healing process for the crack even during a loading phase as demonstrated in [7].

Here we report on the first attempt at introducing a dual fracture/healing mechanism in a rational description of fracture evolution. Admittedly, we can only do so in the most simplistic (oversimplistic?) setting, that of a e.g. two-dimensional scalar field with quadratic internal energy; further we assume that both cracking and healing are rate independent and that the corresponding loss, or gain of surface energy is proportional to the length of the added, or reduced part of the crack. This is clearly too naive on several grounds: first we have thrown away the all important impact of finite deformation and, even more so, of incompressibility. Then, it is highly dubious that either the cracking, or the healing process can be viewed as truly rate-independent in rubber.

In any case, within this framework – which is akin to a A.A. Griffith-type model [4]– we demonstrate the existence of a well posed quasi-static energetic evolution à la A. Mielke [6] under the further topological restriction that the cracks be continua of finite length (compact connected, or maybe with a preset

number of connected components). This is an existence result in the spirit of the original 2d existence result for fracture evolution by G Dal Maso & R. Toader for fracture only [2].

The precise result is as follows:

Theorem 1 (**Quasi-static evolution).** *Let $\Omega \subseteq \mathbb{R}^2$ be open and bounded. Let*

$$c_1 \geq 0, \qquad c_2 > c_3 > 0, \qquad T > 0,$$

and let $g \in AC([0,T]; H^1(\Omega))$ be such that

$$\sup_{t\in[0,T]} \|g(t)\|_\infty < +\infty.$$

Let finally (u_0, K_0) with K continuum, $u_0 \in H^1(\Omega \setminus K)$ and $u_0 = g(0)$ on $\partial\Omega \setminus K$ be a globally stable configuration (i.e., satisfy property (1) below).

Then there exists a mapping $\{t \mapsto (u(t), K(t)) : t \in [0,T]\}$ such that

$$(u(0), K(0)) = (u_0, K_0)$$

and also such that, for every $t \in [0,T]$, the following items hold true.

(a) *Global stability: For every (v,Γ) with Γ continuum and $v \in H^1(\Omega \setminus \Gamma)$, $v = g(t)$ on $\partial\Omega \setminus \Gamma$,*

$$\mathcal{E}(u(t), K(t)) \leq \mathcal{E}(v,\Gamma) + (c_1 - c_2)\mathcal{H}^1(\Gamma \setminus K(t)), \tag{1}$$

where $\mathcal{E}(v,\Gamma) := \int_\Omega |\nabla v|^2 \, dx + c_2\mathcal{H}^1(\Gamma)$.

(b) *Energy balance: $\mathcal{E}(u(t), K(t)) + Diss(0,t) = \mathcal{E}(u(0), K(0)) + 2\int_0^t \nabla u(\tau) \cdot \nabla \dot{g}(\tau)\, dx$ with*

$$Diss(a,b) := (c_1 - c_2) \sup \left\{ \sum_{i=0}^{n} \mathcal{H}^1(K(s_{i+1}) \setminus K(s_i)) : a = s_0 < s_1 < \cdots < s_{n+1} = b \right\}.$$

The method of proof is well known by now: perform a discretisation of size δ in time of the interval of study, write a sequence of minimization problems for the discrete times, interpolate the minimizers with piecewise constant functions and pass to the limit in the size δ of the discretisation. However several hurdles stand in the way of the proof. We will just mention here the lack of monotonicity of the mapping $t \mapsto K_\delta(t)$ for the inclusion which prevents application of any kind of Helly type theorem that would establish the existence of a subsequence δ_n of δ such that $K_{\delta_n}(t) \to K(t)$ for some $K(t)$ for all t's as $n \nearrow \infty$.

References

[1] J. M. Ball. Discontinuous equilibrium solutions and cavitation in nonlinear elasticity. *Philos. Trans. Roy. Soc. London Ser. A*, 306: 557–611, 1982.

[2] G. Dal Maso and R. Toader. A model for the quasi-static growth of brittle fractures: existence and approximation results. *Arch. Ration. Mech. Anal.*, 162(2):101–135, 2002.

[3] A.N. Gent and P.B. Lindley. Internal rupture of bonded rubber cylinders in tension. *Proc. Royal Soc. London, A*, 2: 195–205, 1959.

[4] A.A. Griffith. The phenomena of rupture and flow in solids. *Phil. Trans. Roy. Soc. London*, CCXXI-A:163–198, 1920.

[5] V. Lefèvre, K. Ravi-Chandar, and O. Lopez-Pamies. Cavitation in rubber: An elastic instability or a fracture phenomenon? *Int. J. Fracture*, 192: 1–23, 2015.
[6] A. Mielke. Evolution of rate-independent systems. In A. Dafermos and E. Feireisl, editors, *Evolutionary equations. Vol. II*, Handb. Differ. Equ., pages 461–559. Elsevier/North-Holland, Amsterdam, 2005.
[7] X. Poulain, V. Lefèvre, O. Lopez-Pamies, and K. Ravi-Chandar. Damage in elastomers: nucleation and growth of cavities, micro-cracks, and macro-cracks. *Int. J. Fracture*, 205: 1–21, 2017.
[8] M.L. Williams and R.A. Schapery. Spherical flaw instability in hydrostatic tension. *Int. J. Fract. Mech.*, 1: 64–71, 1965.

Microstructure of dislocations in $3D$

Adriana Garroni
(joint work with S. Conti, A. Massaccesi, S. Müller, M. Ortiz)

The motion of dislocations is considered the main mechanism responsible for plastic flow. Several analytical results describe dislocation dynamics in $2D$, i.e., assuming dislocations to be infinite straight lines in a cylindrical domain, and hence considering point singularities in two-dimensional domains. With this simplifying assumption the problem reduces to the study of the evolution of particles interacting through a logarithmic potential (the so called discrete dislocation dynamics).

In the fully three-dimensional description instead, a leading contribution in the motion of dislocations is played by the line-tension energy, and hence the geometry of the dislocations enters into play and produces relevant effects. In their motion these lines create complex microstructure, as network structures, that influence the effective plastic behavior of the body. The modeling of such microstructures still needs to be understood.

We consider the classical line-tension energy, per unit length, for an infinite straight dislocations (the so called pre-logarithmic factor of the elastic distortion induced by the dislocation). With an asymptotic analysis we then provide a variational formulation the line-tension energy density, $\psi(b,t)$. This depends on the multiplicity b, the Burgers vector, which belongs to the (discrete) set of admissible Burgers vectors $\mathcal{B}$ (e.g., $\mathbb{Z}^3$ if the underlining lattice is cubic), and on the direction t of the line.

A given distribution of dislocations in a domain Ω can be represented by a divergence-free matrix-valued measure supported on curves, i.e. a measure of the form

$$\mu = \theta \otimes \tau \, \mathcal{H}^1 \llcorner \gamma \,, \tag{1}$$

where $\theta : \Omega \subset \mathbb{R}^3 \to \mathcal{B}$ is the multiplicity, γ is a 1-rectifiable set and τ its tangent vector, satisfying $\mathrm{div}\mu = 0$, i.e. $\int_\Omega \varphi \, d\mu = 0$ for all $\varphi \in C^1_0(\Omega, \mathbb{R}^3)$.

In [3], by means of an asymptotic analysis in terms of Γ-convergence of the regularised scaled elastic energy we deduce the line tension energy associated to a

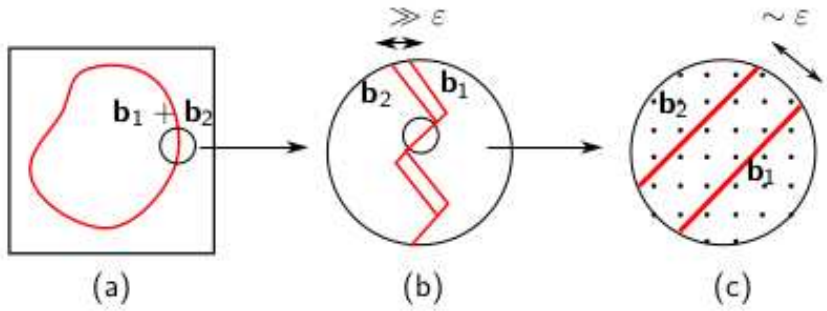

FIGURE 1. Multiscale relaxation of the dislocation energy. (a) shows a macroscopic dislocation line, whose energy per unit length is characterized by ψ^{rel}. (b) illustrates a blow-up of a small portion of that dislocation, which - in this example - exhibit a microstructure. These lines are very close on the scale of the sample, so that they are not distinguished in (a). A single line at the scale of (b) are two separate dislocation lines at the scale of the lattice in (c), which illustrates a further blow-up.

given distribution of dislocations

$$\int_\gamma \psi^{\mathrm{rel}}(\theta,\tau)\, d\mathcal{H}^1 \,. \tag{2}$$

The local effective line tension energy density ψ^{rel} is obtained through a relaxation procedure that may lead to the formation of microstructure as illustrated in Figure 1 (see also [2]).

The next step is to start from the line tension energy and deduce a macroscopic energy depending on a density of dislocations which is obtained in the limit as the number (or total length) of dislocations increases (tends to infinity). To this end we restrict our attention to the case in which all line dislocations are confined to a given slip plane. This simplification allows to represent dislocations in an alternative framework, to that of two-dimensional Caccioppoli partitions ([1]), interpreting them as discontinuities of a phase field $u \in BV(\Sigma,\mathbb{Z}^2)$, with $\Sigma \subseteq \mathbb{R}^2$, representing the slip along Σ, and hence the line tension energy reads

$$E(u) = \int_{J_u} \psi^{\mathrm{rel}}([u],\nu_u^\perp)\, d\mathcal{H}^1 \,, \tag{3}$$

where $[u] := u^+ - u^-$ denotes the jump of u and ν_u the normal to the jump set J_u of u. We therefore introduce a small parameter $\sigma > 0$ and consider the following rescaled energy

$$E_\sigma(v) = \int_{J_v} \sigma\psi^{\mathrm{rel}}\left(\frac{[v]}{\sigma},\nu_v^\perp\right) d\mathcal{H}^1 \,, \qquad v \in BV(\Sigma,\sigma\mathbb{Z}^2)\,. \tag{4}$$

In [4] we prove that the Γ-limit of this energy is the following effective macroscopic model for plasticity

$$E_0(v) = \int_\Sigma g\left(\frac{Dv}{|Dv|}\right)|Dv|\,, \qquad v \in BV(\Sigma, \mathbb{R}^2)\,, \tag{5}$$

where the plastic slip field v has lost the crystallographic constraint. The energy density g is determined by a cell-problem formula and it is obtained by means of a further relaxation process. In the case of cubic crystals with isotropic elasticity, for instance, we show that complex microstructures may form, in which dislocations with different Burgers vector and orientation interact with each other to reduce the total self energy (as illustrated in Figure 2).

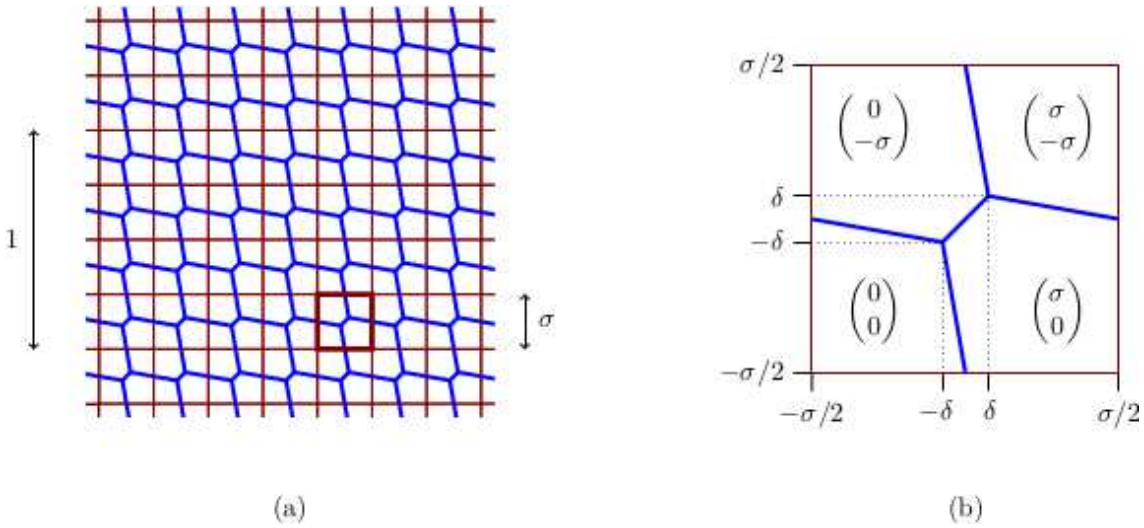

FIGURE 2. Sketch of the microstructure for the cubic lattice and the average dislocation distribution $A = e_1 \otimes e_2 - e_2 \otimes e_1$ and a finite u which take the values 0, $\binom{\sigma}{0}$, etc. Reprinted from [5, Fig. 6] with permission from Elsevier.

Starting from a vectorial phase-field Nabarro-Peierls model introduced by Ortiz and coworkers [6, 7], in the limit of small lattice spacing, we show that, in a scaling regime where the total length of the dislocations is large, the phase-field model reduces to a simpler model of the strain-gradient type. The limiting model contains a term describing the three-dimensional elastic energy and a strain-gradient term describing the energy of the geometrically necessary dislocations, characterized by the tangential gradient of the slip v. The energy density appearing in the strain-gradient term is exactly the function g given by (5) which may give rise to dislocation network-like structures.

References

[1] Ambrosio L., Braides A.: *Functionals defined on partitions in sets of finite perimeter. II. Semicontinuity, relaxation and homogenization*, J. Math. Pures Appl. (9) 69 (1990), 307–333.

[2] Conti S., Garroni A., Massaccesi A.: *Modeling of dislocations and relaxation of functionals on 1-currents with discrete multiplicity*, Calc. Var. Partial Differential Equations, 54, no. 2 (2015), 1847-1874

[3] Conti S., Garroni A., Ortiz M.: *The line-tension approximation as the dilute limit of linear-elastic dislocations*, Arch. Rational Mech. Anal., 218, no. 2 (2015), 699–755.

[4] Conti S., Garroni A., Müller S.: *Homogenization of vector-valued partition problems and dislocation cell structures in the plane*, Boll. Unione Mat. Ital. 10, no. 1 (2017), 3?17.

[5] Conti S., Garroni A., Müller S.: *Dislocation microstructures and strain-gradient plasticity with one active slip plane*, J. Mech. Phys. Solids 93 (2016), 240–251.

[6] Koslowski M., Cuitino A. M., and Ortiz M.: *A phase-field theory of dislocation dynamics, strain hardening and hysteresis in ductile single crystal*, J. Mech. Phys. Solids, 50 (2002), 2597–2635,.

[7] Koslowski M., Ortiz M.: *A multi-phase field model of planar dislocation networks*, Model. Simul. Mat. Sci. Eng., 12 (2004) 1087–1097.

Construction of rank-one convex non-quasiconvex functions of high symmetry

Yury Grabovsky

A central concept in modern Calculus of Variations is quasiconvexity, introduced by C.B. Morrey in 1952 [10] as a criterion of sequential weak-* lower semi-continuity. The same condition is also a necessary condition for a vector field $\boldsymbol{u}(\boldsymbol{x})$ to be a strong local minimizer of the energy functional

$$E[\boldsymbol{u}] = \int_\Omega W(\nabla \boldsymbol{u}) d\boldsymbol{x}.$$

This condition is Jensen's inequality but only for gradients

$$\int_{\mathbb{R}^d} \{W(\boldsymbol{F} + \nabla \boldsymbol{\phi}) - W(\boldsymbol{F})\} d\boldsymbol{x} \geq 0$$

for every $\boldsymbol{\phi} \in C_0^\infty(\mathbb{R}^d; \mathbb{R}^m)$.

An early attempt to understand the true meaning of this concept was to decide if it was equivalent to rank-one convexity. The question remained opened until Šverák settled it in 1992 [11], giving an example of a Lagrangian defined on 3x2 matrices, that is rank-one convex, but not quasiconvex. The example is a polynomial function with no apparent symmetries.

There is also a parallel question about the effective behavior of composite materials, whether every composite can be mimicked by a laminate made with the same set of constituent materials. This question has also been answered in the negative, by Milton [9, Sections 31.8–9], who exploited Šverák's construction and a well-known connection between G-closed sets and quasiconvex functions and L-closed sets (sets containing effective tensors of all laminates made from materials taken from that set) and rank-one convex functions.

Exploiting the relation with the theory of composites in the opposite direction is seemingly more difficult, as we place more restrictions on possible density functions $W(\boldsymbol{F})$. In this talk a new example of a rank-one convex, non-quasiconvex function with a very large group of symmetries is constructed. This example comes from the theory of exact relations - formulas that hold for effective tensors of all composites made with a given set of materials, regardless of the microstructure. The algebraic nature of the theory, developed in collaboration with Graeme Milton [6], is responsible for the aesthetic beauty of the new example. In this example the vector field $\boldsymbol{u}$ is defined on $\mathbb{R}^2$ with values in $\mathbb{R}^8$, represented as a direct sum of two copies of quaternions $\mathbb{H}$: $\mathbb{R}^8 \cong \mathbb{H}^2$. So that

$$W(\nabla \boldsymbol{u}) = \sqrt{\left\|\frac{\partial \boldsymbol{u}}{\partial x}\right\|_{\mathbb{H}^2}^2 \left\|\frac{\partial \boldsymbol{u}}{\partial y}\right\|_{\mathbb{H}^2}^2 - \left|\left(\frac{\partial \boldsymbol{u}}{\partial x}, \frac{\partial \boldsymbol{u}}{\partial y}\right)_{\mathbb{H}^2}\right|^2}, \tag{1}$$

This function is rank-one convex, but not quasiconvex: $QW(\boldsymbol{I}_2) < W(\boldsymbol{I}_2)$, where $\boldsymbol{I}_2$ is the quaternionic 2×2 identity matrix. Compared to Šverák's 3×2 example, this 8×2 example is higher-dimensional. Instead, it has a very large group of symmetries

- $W(\lambda \boldsymbol{F}) = \lambda^2 W(\boldsymbol{F}), \quad \forall \lambda \in \mathbb{R}$
- $W(\boldsymbol{F}\boldsymbol{R}) = W(\boldsymbol{F}) \quad \forall \boldsymbol{R} \in O(2, \mathbb{R})$
- $V(\boldsymbol{G}\boldsymbol{Q}) = V(\boldsymbol{G}) \quad \forall \boldsymbol{Q} \in Sp(2) \cong U(2, \mathbb{H}) = \{\boldsymbol{Q} \in \mathbb{H}^{2\times 2} : \boldsymbol{Q}\boldsymbol{Q}^H = \boldsymbol{I}_2\}$

In order to produce such an example we consider 2D multifield periodic composite materials, whereby n curl-free fields $(\nabla\phi_1, \ldots, \nabla\phi_n)$ are coupled to n, divergence-free fields $(\boldsymbol{j}_1)$:

$$\nabla \cdot \mathsf{L}\left(\frac{\boldsymbol{x}}{\epsilon}\right) \nabla \boldsymbol{\phi} = 0,$$

where $\mathsf{L}(\boldsymbol{z})$ is $[0,1]^2$-periodic L^∞ tensor fields with values in $\mathrm{Sym}^+(\mathbb{R}^{n\times 2})$. A submanifold $\mathbb{M} \subset \mathrm{Sym}^+(\mathbb{R}^{n\times 2})$ of positive codimension is called an exact relation, if the effective tensor L^* of an *arbitrary* composite made with materials taken from $\mathbb{M}$ must necessarily be in $\mathbb{M}$. The idea is to test this property by laminar microstructures. This results in a surprisingly beautiful algebraic characterization of all such submanifolds [6, 5]. Specifically, they are diffeomorphic images of Jordan $\mathcal{A}$-multialgebras—subspaces Π in $\mathrm{Sym}^+(\mathbb{R}^{n\times 2})$ closed with respect to a family of Jordan multiplications, parametrized by a subspace $\mathcal{A}$:

$$\mathsf{K}_1 *_{\mathsf{A}} \mathsf{K}_2 = \frac{1}{2}(\mathsf{K}_1\mathsf{A}\mathsf{K}_2 + \mathsf{K}_2\mathsf{A}\mathsf{K}_1) \in \Pi, \quad \forall \{\mathsf{K}_1, \mathsf{K}_2\} \subset \Pi,\ \mathsf{A} \in \mathcal{A}. \tag{2}$$

In our context $\mathcal{A} = \{\boldsymbol{I}_n \otimes \boldsymbol{A} : \boldsymbol{A} \in \mathrm{Sym}(\mathbb{R}^2),\ \mathrm{Tr}\,\boldsymbol{A} = 0\}$. The final fundamental ingredient is supplied by an algebraic condition that is necessary of Π to correspond to an exact relation, but which is not a consequence of (2). This condition, discovered in [4] (see also [5, 3]) is called the 3-chain condition: $\mathsf{K}_1\mathsf{A}_1\mathsf{K}_2\mathsf{A}_2\mathsf{K}_3 + \mathsf{K}_3\mathsf{A}_2\mathsf{K}_2\mathsf{A}_1\mathsf{K}_1 \in \Pi$, for any $\{\mathsf{K}_1, \mathsf{K}_2, \mathsf{K}_3\} \subset \Pi$ and $\{\mathsf{A}_1, \mathsf{A}_2\} \subset \mathcal{A}$. An analogous 4-chain condition is sufficient for Π to correspond to an exact relation. It is a theorem of Cohn [2] that 2,3 and 4-chain properties are equivalent to "reflexivity" of the Jordan multialgebra. Namely, a reflexive Jordan multialgebra Π

is exactly the set of all symmetric operators in a smallest associative multialgebra Π', containing Π.

The guidance for identifying non-reflexive algebras was obtained by examining reflexivity of all Jordan subalgebras in $\mathrm{Sym}(\mathbb{R}^n)$, characterized in [1]. It turns out that all the nonreflexive Jordan subalgebras in $\mathrm{Sym}(\mathbb{R}^n)$ are "spin factors" [8], whose explicit construction is based on the algebra of quaternions. Once, one knows what to look for, the non-reflexive example in $\mathrm{Sym}(\mathbb{R}^{4\times 2})$ is easy to find, where $n = 4$ corresponds precisely to the identification of $\mathbb{R}^4$ with the algebra of quaternions. The non-reflexive algebra Π gives rise to a submanifold $\mathbb{M}$ that contains all effective tensors of laminates made with material in $\mathbb{M}$, but is not an exact relation. Using variational formulation of the theory of composite materials [7], we produce a family of rank-one convex, non-quasiconvex functions, of which (1) is an example. For full discussion see [3].

References

[1] J.-L. Clerc. Représentation d'une algèbre de Jordan, polynômes invariants et harmoniques de Stiefel. *Journal für die reine und angewandte Mathematik*, 423:47–72, 1992.

[2] P. M. Cohn. On homomorphic images of special Jordan algebras. *Canadian J. Math.*, 6:253–264, 1954.

[3] Y. Grabovsky. From microstructure-independent formulas for composite materials to rank-one convex, non-quasiconvex functions. to appear in Arch. Rat. Mech. Anal.

[4] Y. Grabovsky. Algebra, geometry and computations of exact relations for effective moduli of composites. In G. Capriz and P. M. Mariano, editors, *Advances in Multifield Theories of Continua with Substructure*, Modeling and Simulation in Science, Engineering and Technology, pages 167–197. Birkhäuser, Boston, 2004.

[5] Y. Grabovsky. *Composite materials: Mathematical theory and exact relations*. IOP Expanding Physics. IOP publishing, Ltd., Bristol, UK, 2016.

[6] Y. Grabovsky, G. W. Milton, and D. S. Sage. Exact relations for effective tensors of polycrystals: Necessary conditions and sufficient conditions. *Comm. Pure. Appl. Math.*, 53(3):300–353, 2000.

[7] R. V. Kohn and G. Strang. Structural design, optimization, homogenization, and relaxation of variational problems. In R. Burridge, G. Papanicolaou, and S. Childress, editors, *Macroscopic Properties of Disordered Media*, volume 154 of *Lect. Notes Phys.*, pages 131–147. Springer-Verlag, 1982.

[8] K. McCrimmon. *A taste of Jordan algebras*. Springer, 2004.

[9] G. W. Milton. *The theory of composites*, volume 6 of *Cambridge Monographs on Applied and Computational Mathematics*. Cambridge University Press, Cambridge, 2002.

[10] C. B. Morrey, Jr. Quasi-convexity and the lower semicontinuity of multiple integrals. *Pacific J. Math.*, 2:25–53, 1952.

[11] V. Šverák. Rank-one convexity does not imply quasiconvexity. *Proc. Roy. Soc. Edinburgh Sect. A*, 120(1-2):185–189, 1992.

The Topological Character of Smectic Liquid Crystals

Randall D. Kamien

Though the systematic use of topology to understand defects in ordered matter is now nearly 50 years old, the original work failed to completely characterize systems with broken translational order, *i.e.*, crystals. Smectics are the simplest

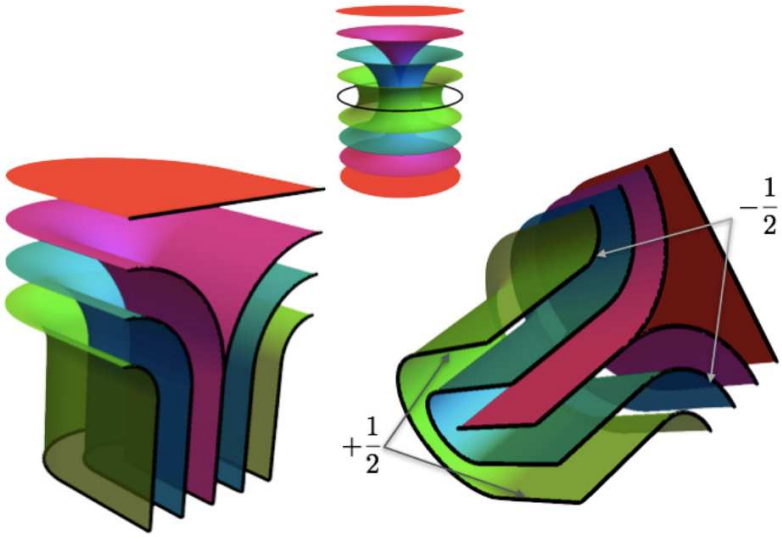

FIGURE 1. Converting a $+\frac{1}{2}$ disclination into a $-\frac{1}{2}$ disclination. The top center shows a toric focal conic domain inserted into an otherwise unperturbed smectic. Topologically, it is point defect in the center surrounded by a $+\frac{1}{2}$ disclination loop. The cylindrical region can attach to equally-spaced planes going off to infinity. If we cut this into four by slicing through a vertical plane and a perpendicular horizontal plane, we can use the quarter toric domain to attach a $+\frac{1}{2}$ disclination into $-\frac{1}{2}$ disclination as shown on the bottom left and right.

example of crystals and we have employed new mathematical tools to study and classify the allowed point and line defects in them. The theory reduces to the time-honored homotopy theory if we ignore the periodic order of the smectic but offers a refinement – though the smectic can support all the defect structure and algebra of the nematic phase that sits above it, the defects have further structure that we have uncovered. This has allowed us to understand previously open puzzles, including the nature of composite dislocations in smectics.

In particular, dislocations are, by their nature, not only topological but *geometrical*: by definition, they only occur in systems with broken translational order and therefore they must induce strain in the crystal or liquid crystal that host them [1, 2, 3]. These strains can grow quite large and often require a cutoff at the core to keep the energy finite. In exchange, the core melts into a higher-symmetry phase bringing with it the higher energy of the uncondensed condensate. Screw dislocations are especially troublesome because of a geometric consequence of their topology. Namely, the helicoidal layer structure that makes up the screw dislocation is not measured at its core [4], that is, all the layers come together on the centerline. It follows that the compression energy must diverge there [5, 6]. The symmetry of the smectic phase allows the core regions of a dislocation to be replaced by disclination pairs, for both edge and screw [7, 8, 9, 10] dislocations. We

will discuss the necessary topology of how an edge dislocation becomes a screw dislocaton through allowed topological and geometrical moves [11].

References

[1] M. Kléman, *Points, Lines and Walls: In Liquid Crystals, Magnetic Systems and Various Ordered Media*, (John Wiley & Sons, New York, 1983).
[2] N.D. Mermin, Rev. Mod. Phys. **51**, 591-648 (1979).
[3] B.G. Chen, G.P. Alexander, and R.D. Kamien, Proc. Natl. Acad. Sci. **106**, 15577 (2009).
[4] V. Poénaru, Commun. Math. Phys. **80**, 127 (1981).
[5] E.A. Matsumoto, C.D. Santangelo, R.D. Kamien, Interface Focus **2** 617 (2012).
[6] R.D. Kamien and T.C. Lubensky, Phys. Rev. Lett. **82** 2892 (1999).
[7] C. E. Williams, Philos. Mag. **32**, 313 (1975).
[8] C. Meyer, Y. Nastishin and M. Kléman, Phys. Rev. E **82**, 031704 (2010).
[9] M.F. Achard, M. Kléman, Y. A. Nastishin, and H. T. Nguyen, Eur. Phys. J. E **16**, 37 (2005).
[10] M. Kléman and O.D. Lavrentovitch, *Soft Matter Physics: An Introduction*, (Springer-Verlag, New York, 2003).
[11] H. Aharoni, T. Machon, and R.D. Kamien, Phys. Rev. Lett. **118**, 257801 (2017).

A geometric theory of homogenization of singular defects

Raz Kupferman

(joint work with Cy Maor)

The modeling of defects in solids has a long ongoing history. One approach, which goes back to the early 1900s, views defects as geometric singularities in locally-Euclidean manifolds. Another approach, dating from the 1950s, models continuously-distributed defects as smooth manifolds endowed with extra fields representing the defects. In this lecture, the two approaches are reconciled. It will be shown that the continuum models of defects are genuine limits of singular defects as their density tends to infinity. By introducing a notion of weak convergence, we show how torsion arises as a homogenization limit of manifolds with distributed singular dislocations, and similarly, how non-metricity arises a homogenization limit of manifolds with distributed point defects.

References

[1] R. Kupferman and C. Maor, *A Riemannian approach to the membrane limit in non-Euclidean elasticity*, *Comm. Contemp. Math.* **16** (2014) 1350052.
[2] R. Kupferman, M. Moshe and J.P. Solomon, *Metric description of defects in amorphous materials*, *Arch. Rat. Mech. Anal.* **216** (2015) 1009–1047.
[3] R. Kupferman and C. Maor, *The emergence of torsion in the continuum limit of distributed dislocations*, *J. of Geom. Mech.* **7** (2015) 361–387
[4] R. Kupferman and C. Maor, *Riemannian surfaces with torsion as homogenization limits of locally-Euclidean surfaces with dislocation-type singularities*, *Proc. Roy. Soc. Edin.* **146A** (2016) 741–768.
[5] R. Kupferman and C. Maor, *Limits of elastic models of converging Riemannian manifolds*, *Calc. Variations and PDEs* **55** (2015) 1–22 .
[6] R. Kupferman, C. Maor and R. Rosenthal, *Non-metricity in the continuum limit of randomly-distributed point-defects*, *Israel J. Math* (in press).

Nonlinear plastic modes

Edan Lerner

Understanding the yielding transition observed upon deforming a glass beyond its elastic limit requires the proper identification of the micro-mechanical objects, akin to dislocations in crystals, that carry plastic flow. In my talk I will introduce a theoretical framework [1] within which a robust, micro-mechanical definition of precursors to plastic instabilities in glassy solids, often termed 'soft-spots', naturally emerges. They are shown to be collective displacements $\hat{\pi}$, referred to here as 'plastic modes', that lead to transitions over energy barriers in the glass. I will demonstrate how plastic modes can be calculated without resorting to conventional harmonic eigenmode analyses, but instead by properly accounting for nonlinearities of the potential energy landscape. I will then show how a heuristic search for nonlinear plastic modes in athermally deformed glassy solids can a-priori detect the locus and geometry of imminent plastic instabilities with remarkable accuracy, at strains as large as $\gamma_c - \gamma \sim 10^{-2}$ away from an instability strain γ_c. Finally, I will introduce the theoretical framework [2] which allows for the rigorous derivation of an equation of motion that describes both the coupling of plastic modes to external deformation, and the resulting mechanical destabilization process, and validate these using numerical simulations of model glasses. These findings suggest that the a-priori detection of the soft-spots field in model glasses can be effectively carried out by a nonlinear plastic modes analysis.

References

[1] L. Gartner and E. Lerner, *Nonlinear plastic modes in disordered solids*, Phys. Rev. E **93**, 011001(**R**) (2016).
[2] E. Lerner, *The micromechanics of nonlinear plastic modes*, Phys. Rev. E **93**, 053004 (2016).

Effective multipole expansion in random media

Felix Otto
(joint work with Peter Bella, Arianna Giunti)

Given a heterogeneous medium as described by a uniformly elliptic (symmetric) coefficient field $a(x)$ in d-dimensional space $\mathbb{R}^d$, and a vector field g supported in the unit ball $B_1(0)$ around the origin, we are interested in the Lax-Milgram solution u of

$$-\nabla \cdot a\nabla u = \nabla \cdot g. \tag{1}$$

Is it possible to predict the field $-\nabla u|_{B_1(y)}$ in the neighborhood of some far-away point y (i.e. with $|y| \gg 1$) without knowing the medium away from 0 and y? In full generality, this is of course not possible. In case of a well-behaved random medium, this however is possible to some extent: For $d = 3$, an effective dipole and quadrupole, but not octupole, can be inferred to high precision just knowing the realization a of the medium in a large, but order-one neighborhood of 0 and y. By

well-behaved, we understand that the ensemble is like in quantitative stochastic homogenization: stationary with correlations of integrable tails.

In case of a homogeneous medium, i.e. a constant coefficient $a \equiv a_h$, by expanding the fundamental solution G_h in the representation formula, i.e.

$$u(y) = G_h(y) \int f dx - \nabla G_h(y) \cdot \int x f dx + \frac{1}{2} \nabla^2 G_h(y) : \int x \otimes x f dx + \cdots$$

where $f := \nabla \cdot g$, the far-field behavior of u in terms of the monopole G_h, the dipole ∇G_h, the quadrupole $\nabla^2 G_h$ etc, can be inferred from the corresponding moments $\int f dx = 0$, $-\int x f dx = \int g$ etc.

In case of a heterogeneous medium, the substitute for the multipoles are the quotient spaces of decaying a-harmonic functions (i.e. functions satisfying $-\nabla \cdot a \nabla u = 0$):

$$Y_k := \left\{ u \text{ } a\text{-harmonic in } \mathbb{R}^d \setminus B_1(0) : \limsup_{|y| \uparrow \infty} |y|^{(d-1)+k} \left(\int_{B_1(y)} |\nabla u|^2 \right)^{\frac{1}{2}} < \infty \right\};$$

we note that in the homogeneous case, Y_k^h / Y_{k+1}^h is indeed spanned by the k-th derivatives of G_h. Furthermore, the substitute for the (homogeneous) polynomials defining the moments are (quotient) spaces of growing a-harmonic functions:

$$X_m := \left\{ v \text{ } a\text{-harmonic in } \mathbb{R}^d : \limsup_{|y| \uparrow \infty} |y|^{-m+1} \left(\int_{B_1(y)} |\nabla v|^2 \right)^{\frac{1}{2}} < \infty \right\};$$

we note that in the homogeneous case, X_m^h / X_{m-1}^h is described by the spherical harmonics of degree m. There is a natural pairing between X_m and Y_k given by

$$\langle v, u \rangle := \int_{\partial B_R} \nu \cdot (va \nabla u - ua \nabla v),$$

an expression that is independent of $R \geq 1$. It is folklore that in the homogeneous case, $\langle \cdot, \cdot \rangle_h$ provides an isomorphism between Y_{k+1}^h / Y_{m+1}^h and the dual space $(X_m^h / X_k^h)^*$ for all $m \geq k \geq 0$.

This isomorphism is a re-expression of the multipole expansion: Indeed from (1) we infer $\langle v, u \rangle_h = \int \nabla v \cdot g$ for all $v \in X_m^h$ so that

$$-\nabla \cdot g \in (X_m^h / X_0^h)^* \cong Y_1^h / Y_{m+1}^h \ni u.$$

Turning to the special case of $m = 2$, this means that the dipole and quadrupole moments of $-\nabla \cdot g$ determine an element of $(X_2^h / X_0^h)^*$, which by the isomorphism identifies an element of Y_1^h / Y_3^h, which in turn is the multipole expansion of u up to quadrupoles. Our main result is that if a_h is the homogenized coefficient, we may construct two isomorphism between X_2^h / X_0^h and X_2 / X_0 and between Y_1^h / Y_3^h and Y_1 / Y_3 that are canonical in the sense that the pairing $\langle \cdot, \cdot \rangle_h$ turns into the pairing $\langle \cdot, \cdot \rangle$.

Theorem 1. [2] *Let $d > 2$ and consider a well-behaved ensemble of uniformly elliptic coefficient fields. Then for almost every realization a, there exist two isomorphisms*

$$v_h \in X_2^h/X_0^h \mapsto X_2/X_0 \ni v, \;\; u_h \in Y_1^h/Y_3^h \mapsto Y_1/Y_3 \ni u \quad s.t. \quad \langle v_h, u_h\rangle_h = \langle v, u\rangle.$$

More precisely, the first isomorphism is of the form

$$v = (1 + \phi_i\partial_i + \psi_{ij}\partial_{ij})v_h \quad \textit{(with summation convention)} \tag{2}$$

and the second isomorphism is characterized by

$$\lim_{|y|\uparrow\infty} |y|^{(d-1)+1+\beta}\left(\int_{B_1(y)} |\nabla(u - (1 + \phi_i\partial_i + \psi_{ij}\partial_{ij})u_h)|^2\right)^{\frac{1}{2}} = 0$$

for any $1 < \beta < \min\{\frac{d}{2}, 2\}$.

A few remarks are in place: A) (2) means that the random functions $\{\phi\}_{i=1,\cdots,d}$ and $\{\psi_{ij}\}_{i,j=1,\cdots,d}$ are the first and second-order correctors, respectively, in the language of homogenization.
B) Coming back to (1); it can be shown that $u \in Y_1$, so that by the theorem there exists $u_h \in Y_1^h$ such that the (second-order) two-scale expansion is close to order β in the sense of

$$\nabla u = \nabla((1 + \phi_i\partial_i + \psi_{ij}\partial_{ij})u_h)(1 + o(|y|^{-\beta})) \quad \text{on } B_1(y)$$

and $u_h \in Y_1^h/Y_3^h \cong (X_2^h/X_0^h)^*$ is characterized by

$$\forall\, v_h \in X_2^h/X_0^h \quad \langle v_h, u_h\rangle_h = \langle v, u\rangle = \int_{B_1(0)} g \cdot \nabla(1 + \phi_i\partial_i + \psi_{ij}\partial_{ij})v_h.$$

Hence in order to infer $\nabla u|_{B_1(y)}$ (to order β), we only need to know the first and second-order correctors in $B_1(y)$ and $B_1(0)$. Those can be approximately inferred by solving $d + \frac{d(d+1)}{2}$ elliptic equations in two representative volume elements around y and 0. Hence indeed, there is no need to know the realization of the medium far away from these two points.
C) An example of a well-behaved ensemble is the following: Given a realization $\{X_n\}_n \subset \mathbb{R}^d$ of the Poisson point process of unit density, consider the isotropic coefficient field a that has value 1 on $\cup_n B_{\frac{1}{4}}(X_n)$ and value $\frac{1}{2}$ on the complement.
D) Why is there a limitation to Y_1/Y_m with $m = 3$, i.e. to quadrupoles, in $d = 3$? This relies on the growth of the correctors: As a rule of thumb, the k-th order corrector grows, up to logarithmic terms, as $|y|^{\max\{k-\frac{d}{2},0\}}$ (very much like the Brownian motion, which can be seen as a first-order corrector in $d = 1$, grows as $|y|^{\frac{1}{2}}$). This means that the order of the homogenization error, no matter how many orders of correctors are included into the two-scale expansion, is limited to $\beta < \frac{d}{2}$. Therefore, $d = 2$ is critical for quadrupoles, $d = 4$ is critical for octupoles etc.

The proof relies on stochastic arguments from [1] establishing that for $d > 2$, ϕ_i is stationary and that ψ_{ij} grows no more than $|y|^{2-\beta}$. It further relies on

deterministic arguments yielding $Y_{k+1}/Y_{m+1} \cong (X_m/X_k)^*$, building upon [3]. The crucial novel part is the argument that $\langle v, u\rangle = \langle v_h, u_h\rangle_h$, which easily reduces to

$$\lim_{R\uparrow\infty} \int_{\partial B_R} \nu \cdot \big((va\nabla\tilde{u} - \tilde{u}a\nabla v) - (v_h a_h \nabla u_h - u_h a_h \nabla v_h)\big) = 0, \tag{3}$$

with $\tilde{u} := (1 + \phi\partial_i + \psi_{ij}\partial_{ij})u_h$ and (2). Since v_h grows as $|y|^2$ and u_h decays only as $|y|^{-d+1}$, we need more than one order of cancellation. A crucial tool consists in complementing the correctors ϕ_i, ψ_{ij} by flux correctors $\sigma_i = \{\sigma_{ijk}\}_{j,k=1,\dots,d}$, $\tau_{ij} = \{\tau_{ijk\ell}\}_{k,\ell=1,\dots,d}$, which are skew-symmetric tensor fields characterized by

$$a(\nabla\phi + e_i) = a_h e_i + \nabla\cdot\sigma_i, \quad a\nabla\psi_{ij} = (\phi_i a - \sigma_i)e_j + C_{hij} + \nabla\cdot\tau_{ij},$$

with C_h a deterministic (1,2)-tensor, and can be shown to have the same growth as ϕ_i and ψ_{ij}, respectively. These allow for the representation of the flux

$$a\nabla\tilde{u} = a_h\nabla u_h + \partial_{ij}u_h C_{hij} + \nabla\cdot(\partial_j u_h \sigma_j + \partial_{ij}u_h\tau_{ij}) + (\psi_{ij}a - \tau_{ij})\nabla\partial_{ij}u_h,$$

from which together with (2) we get to first order (but in a weak topology),

$$va\nabla\tilde{u} \approx v_h a_h\nabla u_h + \phi_i\partial_i v_h a_h\nabla u_h + v_h\partial_{ij}u_h C_{hij} - \partial_i v_h\partial_j u_h\sigma_j(e_i + \nabla\phi_i).$$

Thanks to the normalization of the expectation $\langle\phi_i\rangle = \langle\sigma_{ijk}\rangle = 0$ we have $C_{hijk} = e_j\cdot\langle(\sigma_i\nabla\phi_k - \sigma_k\nabla\phi_i)\rangle$, so that as a consequence of ergodicity

$$\begin{aligned}&(va\nabla\tilde{u} - \tilde{u}a\nabla v) - (v_h a_h\nabla u_h - u_h a_h\nabla v_h)\\ &\approx (v_h\partial_{ij}u_h - u_h\partial_{ij}v_h)C_{hij} + \partial_i v_h\partial_j u_h C_{hi\cdot j}.\end{aligned}$$

The limit (3) then follows via a Null-Lagrangian structure of the above rhs coming from the skew-symmetry of C_{hijk} in (i,k).

References

[1] P. Bella, B. Fehrman, J. Fischer, F. Otto, *Stochastic homogenization of linear elliptic equations: Higher-order error estimates in weak norms via second-order correctors*, to appear in SIAM J. Math. Analysis.

[2] P. Bella, A. Giunti, F. Otto, *Effective multipoles in random media*, arXiv.

[3] J. Fischer, F. Otto, *A higher-order large-scale regularity theory for random elliptic operators*, Comm. Partial Differential Equations **41** (2016), no. 7, 1108–1148.

The Role of Nucleus Stiffness in the Physical Limit of Cell Migration

Luigi Preziosi

(joint work with Chiara Giverso)

The acquisition of the ability of cells to move in the network of fibers they live in and across membranes is a fundamental step not only in cancer invasion and in the spread of metastasisis, but also in physiological processes like wound healing. Therefore, understanding the relevant mechanisms underlying this process has important consequences on conceiving possible actions on the one hand to hamper cancer invasion and on the other hand to speed up healing processes.

For this reason recently many experiments have been performed to understand the mechanisms of cell migration but they were mainly done on flat two-dimensional surfaces. Differently, cell motility in vivo takes place in three-dimensional environments, of course, and biological tests on three-dimensional migration indicate that in such more realistic set-ups cell motion can substantially differ from migration on two-dimensional substrates, since the geometric microscopic characteristics of the extra-cellular matrix (ECM) the cell live in and the cellular lining the cell encounter along their way may constitute steric obstacles to their motion [7, 11, 20].

Indeed, in many cases, the openings in the three-dimensional extracellular environment might be substantially smaller than the cell diameter and therefore when cells encounter such constrictions in the interstitial space, migration requires substantial cellular deformations, to adapt the shape of the cell to the only slightly bendable fibrillar network. In many cases migration even requires the activation of a proteolytic program involving the production of enzymes named matrix metalloproteinases (MMPs) that are able to degrade the fibers of the extra-cellular matrix widening the size of the pores.

Looking more in detail, experiments show that whilst the cytoplasm is very flexible and is able to accommodate nearly any pore size, the cell nucleus is an order of magnitude stiffer than the surrounding cytoplasm and, with a typical diameter of 3-10 μm, might be larger than the spacing among fibers in the ECM [5]. So, stiff nuclei might not be able to squeeze through the narrow pores, defining a critical pore size below which cells remain trapped. This critical pore cross-section was estimated to be in the order of 10% of the original nucleus cross-section and was defined as the *physical limit of migration* [20].

Therefore, in order to penetrate energy need be spent mainly to deform the cell nucleus, so that it is able to pass through the narrow pores. This energetic cost is irrelevant when the cell is migrating in three-dimensional networks with typical distances among fibers larger than the nuclear dimension and, of course it is absent when the cell is crawling on two-dimensional substrata. On the other hand, it increases considerably in realistic three-dimensional set-ups when the spacing available among the fibers is much smaller than the dimension of the nucleus, even becoming prohibitive. In this case nuclear deformation becomes a limiting factor to cell migration [21].

In [8] we estimated the energy required to deform the elastic nuclear membrane and the internal genetic material, described as a neo-Hookean elastic solid, whereas the cytoplasm is treated as an inviscid liquid that can easily adapt to fit any channel size, so that the energetic contribution related to the deformation of the cellular membrane and of its cytoplasm can be neglected. Then we compared this energy with the work that can be performed by the cell to pull itself within the pore network. This energy might be provided both by the cell myosin-actin-focal adhesion machinery and by stress passively acting on the cell (i.e., fluid flow in microfluidic devices or the pressure of surrounding cells in growing multicellular aggregates).

The basic assumption is that, in order to have a cell entering inside a microchannel, the energy needed to deform the nucleus and its membrane should be smaller than the work that could be actively generated by the cell (i.e., through the integrin-mediated cytoskeletal contraction) and passively exerted on the cell (i.e., through stresses acting on the cell). Denoting respectively with W_{active} and $W_{passive}$ these two contributions, the criterium for cell entrance inside a channel reads

$$W_{active} + W_{passive} > W_S + W_V \,, \tag{1}$$

where we distinguished the energy related to membrane extension, W_S, and the one related to bulk compression W_V.

In order to compute the energy required to deform the nucleus some assumptions need be made on the shape acquired by the nucleus to pass through narrow ECM restrictions. Experimental evidences [20] suggest that, when the cell is forced to cross microchannels of sterically limiting geometries, the nucleus acquires an elongated shape oriented along the cell long-axis direction, that resembles an ellipsoid or a sigar with a cylindrical inner part ending with two spherical caps. In [9] it was shown that the difference of energy required to achieve the two configurations is negligible. So, in [8] the initial spherical nucleus of radius R_n is taken to deform into a prolate ellipsoidal nucleus, with minor semi-axes equal to the radius of the channel pore, R_p, preserving the total volume of the nucleus.

Regarding the surface contribution, following [6] the energy that is required to deform the surface area was taken to be

$$W_S = \lambda(\Delta S)(\Delta S)^2 \,, \tag{2}$$

where ΔS is the increase on the surface area passing from an initial spherical shape to the final ellipsoidal configuration and $\lambda(\Delta S)$ can be either constant or an increasing function of ΔS. Actually, it is found that there is a maximum stretched area for the nuclear envelope, due to its lamin network layered below the nuclear membrane. However, more refined relations for the membrane energy might be considered as well as for the bulk genetic material [10, 17, 18, 19]. Nevertheless, using (2) and a neo-Hookean law allows to obtain easy analytical computations and it has been shown to well represent cell behaviour at least in a certain range of deformations [6].

The other relevant component to be evaluated in Eq.(1) is the work done by the traction forces that involve both the formation of integrin mediated adhesion bonds to the extra-cellular matrix (ECM) and actomyosin-mediated contraction to propel the nucleus forward. What is known by traction force microscopy [1, 2, 12] is that traction forces are exerted mainly in the regions close to the head and to the tail of polarized cells and that the traction forces of a single bond is about 10 pN. Thus, in addition to the strength of the traction force F the total force also depends on the density of expressed and activated integrins, ρ_b, over the surface of contact between the cell and the ECM, and on the portion of the surface of contact composed by ECM ligands, α_{ECM}, i.e., the ratio of the channel surface for which the cell can actually bond to the ECM.

It is found that a crucial parameter is the dimensionless number $G = \rho_b \alpha_{ECM} F/\mu$ that compares quantities related to the traction forces at the numerator, with the nucleus stiffness at the denominator. Hence, large G's correspond, for instance, to larger traction forces, better ability to adhere to the substratum, or softer cell nuclei.

In fact, computating the energetic terms in (1) gives the following criterium for the physical limit of migration

$$G < \bar{G} = \frac{a(\tilde{R}_p) + 8\pi\beta b(\tilde{R}_p)}{c(\tilde{R}_p)\tilde{R}_p L(\tilde{R}_p, \tilde{R}_c)}, \tag{3}$$

where

(4)

$$a(\tilde{R}_p) = \frac{2}{3}\tilde{R}_p^2 + \frac{1}{3\tilde{R}_p^4} - 1, \qquad b(\tilde{R}_p) = \left[\frac{\tilde{R}_p^2}{2}\left(1 + \frac{\sin^{-1}\sqrt{1-\tilde{R}_p^6}}{\tilde{R}_p^3\sqrt{1-\tilde{R}_p^6}}\right) - 1\right]^2,$$

$$c(\tilde{R}_p) = \frac{2}{\tilde{R}_p^2} - 1 + \sqrt{1-\tilde{R}_p^6},$$

$$L(\tilde{R}_p, \tilde{R}_c) = \frac{4\tilde{R}_c^3 - 3\tilde{R}_p^2 - 2\tilde{R}_p^3 - 2 + 2(\tilde{R}_p^2 - 1)\sqrt{1-\tilde{R}_p^2}}{3\tilde{R}_p^2}.$$

It can be noticed that the right hand side is a function of the normalized radii $\tilde{R}_p = R_p/R_n$ and only through L of $\tilde{R}_c = R_c/R_n$, in addition to the dimensionless parameter $\beta = \lambda_0 R_n/\mu$.

As sketched in Fig. 1, given a cell of radius R_c with a nucleus of dimension R_n and nuclear mechanical properties, for every diameter ratio $\tilde{R}_p$, it is possible to define the value of G, such that for $G < \bar{G}$ cells cannot enter inside a channel of radius $\tilde{R}_p R_n$.

Hence, knowing the density of expressed and activated integrins ρ_b on the contact surface, the portion of the ECM α_{ECM} available to form bonds, the cytoskeletal traction force F generated by a single bond and, finally, the mechanical properties of the nucleus (i.e., its shear modulus μ and the surface stiffness β), moving on the horizontal line in the graph on the left of Fig. 1 it is possible to identify the minimum cross section of ECM channels that can be penetrated by the cell.

Conversely, knowing the characteristic dimensions of the pores in the ECM, of the cell, and of the nucleus, moving on the vertical line in the graph on the right of Fig. 1 it is possible to identify the minimum value of the parameter G such that the cell might be able to penetrate into the ECM network. For instance, for constant adhesion parameters, this means that the nucleus must be soft enough, i.e., μ below a threshold value, or the traction force must be strong enough, i.e., F above a threshold value. Furthermore, the criterium shows the possibility of clonal selection in a population between moving and non-moving cells, for instance on the basis of the nucleus stiffness or on their traction abilities.

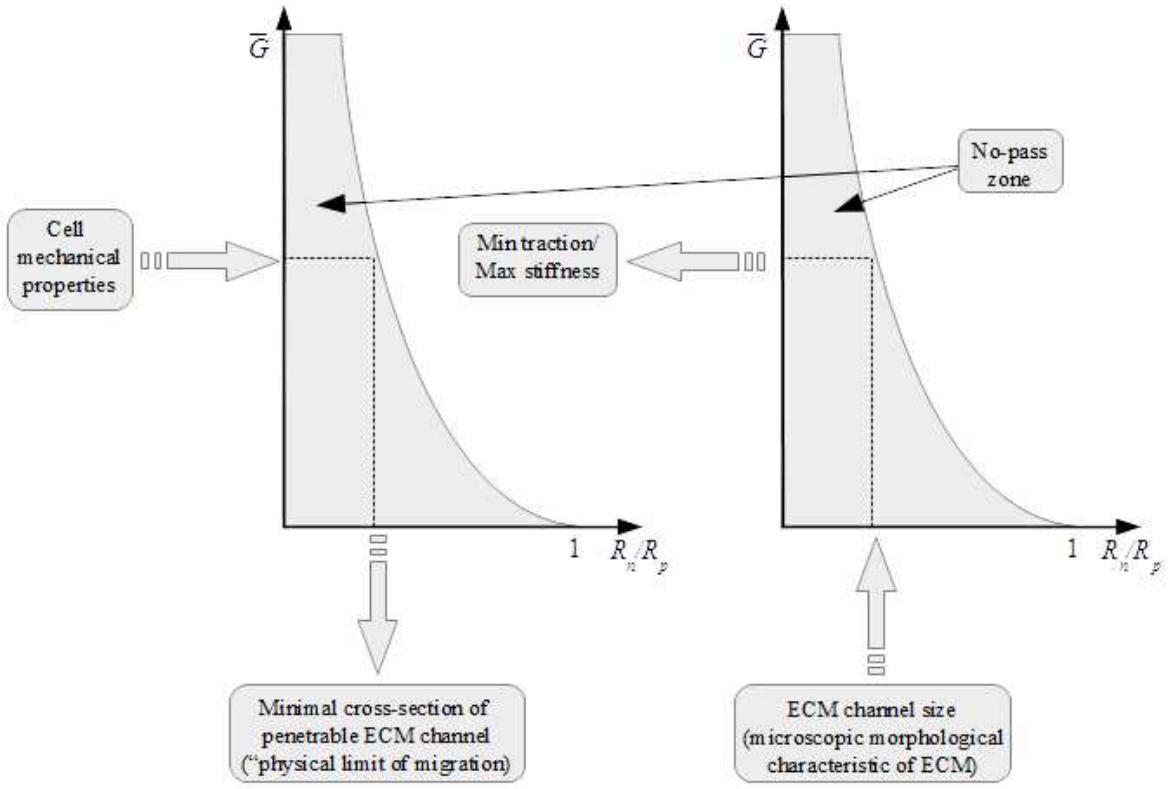

FIGURE 1. Schematic representation of the biological interpretation of the relation between $\bar{G}$ and $\tilde{R}_p = R_p/R_n$ for given cell radius and β. The dashed region corresponds to the region in the parameter space for which the cell cannot enter inside the ECM channel.

This finding is in qualitative agreement with a number of experimental works, such as [4, 13, 21], where cell migratory capability is associated with nuclear deformability. Moreover, it is qualitatively comparable with the results obtained with individual cell-based model [14, 15, 16], confirming that mechanical properties of the nucleus can affect the cell entry into channels.

We also mention that the relation (3) can be of great value, for instance, in scaffold design. Indeed, we can conclude that also in view of the simulations in [14, 15, 16] the optimal pore size to allow the repopulation of cells involved in wound healing, such as fibroblasts and keratocytes, is slightly larger that the dimension of their nucleus.

The same mechanisms outlined in the case of single cell migration inside an ECM channel characterize and limit the invasion of multicellular aggregates while growing in dense ECMs [20]. Indeed, the cells at the border of the cellular spheroid try to penetrate the surrounding fiber network, but, whereas their cytoplasm is able to protrude in the pores of the ECM as observed for single cells, their nuclei might remain trapped at the border of the aggregate, depending on the geometrical (in particular, the typical pore size of the extracellular network) and the mechanical properties of the cells (mainly, the stiffness of the cells' nuclei) [20]. In particular,

when the spheroid is immersed in an ECM network with a pore size that is not sterically restrictive, the cells at the outer border of the spheroid can invade the surrounding collagenous environment. On the other hand, when the pore size in the collagen network is too small (with respect to the nuclear dimension) and the cells in the multicellular aggregate cannot secrete MMPs, the cells cannot invade the surrounding tissue, since their nuclei remain trapped at the border of the spheroid, even though their cytoplasms tend to protrude into the network.

We explicitily mention that it is not the ECM density that plays a role here, but its microstructure, though the two characteristics are of course related. In fact, as it can be readily realized conceptually and obtained experimentally by building the ECM networks at different temperatures, the same ECM density of the fiber network can be achieved with thinner fibers and smaller spacings among them and thicker fibers and larger spacings.

Therefore, keeping in mind the penetration criterium discussed before and in more details in [3] a multiphase model is proposed characterized by the presence of a motility coefficient

$$M = \alpha \frac{(A_m - A_0)_+}{\left(1 + \frac{A_m - A_0}{A_1}\right)^n}, \tag{5}$$

relating the velocity of the cellular constituent to the stress tensor.

In (5) $(f)_+$ stands for the positive part of f, A_m is the typical cross section of the pores in the ECM and A_0 is the critical cross section related to the physical limit of migration. Recalling the discussion above, and coherently with experimental outcomes reported for instance in [20], it is clear that A_0 cannot be constant but should depend on the ratio of the pore size with respect to the nucleus size and through G on the elasticity of the nucleus and of its membrane, on cell adhesion, on cell traction and on compression of the cell aggregate.

The model deduced in this way allows to describe the macroscopic invasion or segregation of multicellular aggregates by thick porous structures, taking into account the limitations imposed by the nuclear envelope and its solid interior material. It can be noticed that from the mathematical point of view the model has an interesting structure because it changes type from parabolic to hyperbolic according to whether A_m is larger than A_0 or not, which from the bio-physical point of view corresponds to the case in which there is penetration in and relative motion with respect to the extra-cellular matrix or not.

References

[1] D. Ambrosi, Cellular traction as an inverse problem. *SIAM J. Appl. Math.* **66**, 2049–2060 (2006).

[2] D. Ambrosi, A. Duperray, V. Peschetola, C. Verdier, Traction patterns of tumor cells. *J. Math. Biol.* **58**, 163–181 (2009).

[3] A. Arduino, L. Preziosi. A multiphase model of tumour segregation in situ by a heterogeneous extra-cellular matrix. *Int. J. Nonlinear Mech.* **75**, 22–30 (2015).

[4] C. Beadle, M.C. Assanah, P. Monzo, R. Vallee, S.S. Rosenfeld, P. Canoll. The role of myosin II in glioma invasion of the brain. *Mol. Biol. Cell.* **19**, 3357–3368 (2008).
[5] P.M. Davidson, C. Denais, M.C. Bakshi, J. Lammerding, Nuclear deformability constitutes a rate-limiting step during cell migration in 3-D environments. *Cell. Mol. Bioeng.* **7**, 293–306 (2014).
[6] E.A. Evans, R. Waugh, L. Melnik, Elastic area compressibility modulus of red cell membrane. *Biophys. J.* **16**, 585–595 (1976).
[7] P. Friedl, K, Wolf, J. Lammerding, Nuclear mechanics during cell migration. *Curr. Opin. Cell. Biol.* **23**, 55–64 (2011).
[8] C. Giverso, A. Arduino, L. Preziosi, How nucleus mechanics and ECM topology influence the invasion of single cells and multicellular aggregates. *Bull. Math. Biol.* in press (doi.org/10.1007/s11538-017-0262-9)
[9] C. Giverso, A. Grillo, L. Preziosi, Influence of nucleus deformability on cell entry into cylindrical structures. *Biomech. Model. Mechanobiol.* **13**, 481–502 (2014).
[10] W. Helfrick, Elastic properties of lipid bilayers: theory and possible experiments. *Z. Naturforsch.* **28**, 693–703 (1973).
[11] P. Isermann, J. Lammerding, Nuclear mechanics and mechanotransduction in health and disease. *Curr. Biol.* **23**, R1113–R1121 (2013).
[12] V. Peschetola, V.M. Laurent, A. Duperray, R. Michel, D. Ambrosi, L. Preziosi, C. Verdier, Time-dependent traction force microscopy for cancer cells as a measure of invasiveness. *Cytoskeleton* **70**, 201–214 (2013).
[13] C. G. Rolli, T. Seufferlein, R. Kemkemer, J. P. Spatz. Impact of tumor cell cytoskeleton organization on invasiveness and migration: a microchannel-based approach. *PLoS ONE* **5**, e8726 (2010).
[14] M. Scianna, L. Preziosi, K. Wolf, A Cellular Potts Model simulating cell migration on and in matrix environments. *Math. Biosci. Engng.* **10**, 235–261 (2013).
[15] M. Scianna, L. Preziosi, Modeling the influence of nucleus elasticity on cell invasion in fiber networks and microchannels. *J. Theor. Biol.* **317**, 394-406 (2013).
[16] M. Scianna, L. Preziosi, A cellular Potts model for the MMP-dependent and -independent cancer cell migration in matrix microtracks of different dimensions. *Comp. Mech.* **53**, 485–497 (2014).
[17] R. Skalak, A. Tozeren, R.P. Zarda, S. Chien,. Strain energy function of red blood cell membrane. *Biophys. J.* **13**, 245–264 (1973).
[18] Z.C. Tu, Z.C. Ou-Yang, Geometric theory on the elasticity of bio-membranes. *J. Phys. A* **37**, 11407–11429 (2004).
[19] Z.C. Tu, Z.C. Ou-Yang, Elastic theory of low-dimensional continua and its applications in bio- and nano-structures. *J. Comput. Theor. Nanosci.* **5**, 422–448 (2008).
[20] K. Wolf, M. te Lindert, M. Krause, S. Alexander, J. te Riet, A.L. Willis, R.M. Hoffman, C.G. Figdor, S.J. Weiss, P. Friedl, Physical limits of cell migration: Control by ECM space and nuclear deformation and tuning by proteolysis and traction force. *J. Cell Biol.* **201**, 1069–1084 (2013).
[21] K. Wolf, Y.I. Wu, Y. Liu, J. Geiger, E. Tam, C. Overall, M.S. Stack, P. Friedl, Multistep pericellular proteolysis controls the transition from individual to collective cancer cell invasion. *Nat. Cell. Biol.* **9**, 893–904 (2007).

The equilibrium measure for a nonlocal dislocation energy

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(joint work with Maria Giovanna Mora and Luca Rondi)

In this talk I presented the recent results in [5] on the characterisation of the equilibrium measure for a nonlocal and *anisotropic* weighted energy describing the interaction of positive dislocations in the plane.

More precisely, in [5] we consider the interaction energy

$$I(\mu) = \iint_{\mathbb{R}^2\times\mathbb{R}^2} V(x-y)\,d\mu(x)\,d\mu(y) + \int_{\mathbb{R}^2} |x|^2\,d\mu(x) \tag{1}$$

defined on probability measures μ representing the mesoscopic dislocation density, where the interaction potential V is given by

$$V(x) = -\log|x| + \frac{x_1^2}{|x|^2}, \qquad x = (x_1, x_2), \tag{2}$$

and corresponds to positive edge dislocations with Burgers vector $\mathbf{e_1}$, and the second term in the energy acts as a confinement.

The minimisers of I describe the equilibrium dislocation patterns at the mesoscale. Although such minimisers have not been characterised analytically so far, neither at the micro nor at the mesoscale, they are conjectured to be vertical wall-like structures (see, e.g., [1, 3]). This belief has triggered a considerable interest in dislocation walls in the engineering and mathematical literature, and interactions, upscaled behaviour and dynamics of walls have been thoroughly analysed.

In [5] we give a positive answer to the conjecture. We prove that the minimiser of I exists, is unique, and is given by a *one-dimensional, vertical* measure, namely the semi-circle law on the vertical axis

$$m_1 := \frac{1}{\pi}\delta_0 \otimes \sqrt{2-x_2^2}\,\mathcal{H}^1 \llcorner (-\sqrt{2},\sqrt{2}).$$

This is the first example of an anisotropic kernel for which the minimiser can be explicitly computed. Even in the radially symmetric case, the explicit characterisation of the equilibrium measure has been done only for the Coulomb potential in any dimension, for the logarithmic potential in dimension one and for power laws.

In two dimensions the Coulomb potential, namely $V_{\mathrm{C}} = -\log|\cdot|$, arises in a variety of contexts, such as, e.g., Fekete sets, orthogonal polynomials, random matrices, Ginzburg-Landau vortices, Coulomb gases. For the same confinement term as in (1), the minimiser is given by the circle law $m_0 := \frac{1}{\pi}\chi_{B_1(0)}$ (see, e.g., [2, 6], and the references therein). Although the radial component of the potential in (2) is exactly the Coulomb kernel V_{C}, the presence of the additional anisotropic term has a dramatic effect on the structure of the equilibrium measure. Unlike m_0, the support of m_1 is one-dimensional and its density is not constant.

For the logarithmic potential in one dimension, corresponding to the so-called Log-gases energy (see, e.g., [4]), Wigner proved in [7] that the semi-circle law is

the unique minimiser. We note that the functional I in (1) coincides with the Log-gases energy on measures with support on the vertical axis, since the anisotropic term vanishes on those measures. Therefore if one could prove that the minimiser of I is supported on the vertical axis, then the minimality of the semi-circle law would follow directly.

This is however not the strategy we use in [5]. Our approach consists of two steps: We first prove the strict convexity of I on the class of measures with compact support and finite interaction energy. Strict convexity implies uniqueness of the minimiser and the equivalence between minimality and the Euler-Lagrange conditions for I. As a second step, we show that the semi-circle law satisfies the Euler-Lagrange conditions and hence is the unique minimiser of I.

The proof of both steps is highly non-trivial. We could not rely on the machinery developed in the classical case of purely logarithmic potentials with external fields (see [6]), which is heavily based on $-\log|\cdot|$ being radially symmetric, and on it being the fundamental solution of the Laplace operator, since V is neither. Similarly, although nonlocal energies are widely used and studied in the mathematical community, and the existence of their ground states and their qualitative properties have received great attention in recent years, the potential is typically required to be radially symmetric, or the singularity to be non-critical, so V is not covered by their analysis.

References

[1] F.P. Duda & M. Šilhavỳ, *Dislocation walls in crystals under single slip*, Comput. Methods Appl. Mech. Engrg. **193** (2014), 5385–5409.

[2] O. Frostman, *Potentiel d'équilibre et capacité des ensembles avec quelques applications à la théorie des fonctions*, Thesis, Meddel. Lunds Univ. Mat. Sem. **3** (1935), 1–118.

[3] J.P. Hirth & J. Lothe, *Theory of dislocations.* John Wiley & Sons, 1982.

[4] M.L. Mehta, *Random matrices.* Third edition. Elsevier/Academic Press, 2004.

[5] M. G. Mora, L. Rondi, and L. Scardia, *The equilibrium measure for a nonlocal dislocation energy*, Preprint arXiv:1612.01137, 2016.

[6] E. Saff & V. Totik, *Logarithmic potentials with external fields.* Springer-Verlag, 1997.

[7] E. Wigner, *Characteristic vectors of bordered matrices with infinite dimensions*, Ann. Math. **62** (1955), 548–564.

Existence and Convergence of Solutions of the Boundary Value Problem in Atomistic and Continuum Nonlinear Elasticity Theory

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(joint work with Julian Braun)

The classical connection between atomistic and continuum models of nonlinear elasticity is provided by the Cauchy-Born rule: The continuum stored energy function associated to a macroscopic affine map is given by the energy (per unit volume) of a crystal which is homogeneously deformed with the same affine mapping. In fact, there are two different approaches to a rigorous justification of the Cauchy-Born rule: Variational methods have been used by Friesecke and Theil

[6] and further developed by Conti, Dolzmann, Kirchheim and Müller [4] showing that, under appropriate conditions, the homogeneous Cauchy-Born deformation is indeed a global energy minimizer for affine boundary conditions. In [2] we have shown that in this setting one also has a discrete-to-continuum Γ-convergence result. A different approach has been used by E and Ming [5] (on the flat torus under rather strong smoothness assumptions) and Ortner and Theil [8] (for the whole space problem), which also applies to atomic interaction potentials with physically realistic decay at infinity. The main results in these contributions show that, under appropriate stability conditions, near solutions of the continuum equations of elasticity there always is a discrete solution of the atomistic system.

The main aim of this note is to report on recent results obtained in [3] on the rigorous derivation of a passage from equilibrium configurations of atomistic systems to solutions of the continuum equations of elastostatics for general boundary value problems.

Atomistic systems.

Let $\Omega \subset \mathbb{R}^d$ be a Lipschitz domain, $\varepsilon\mathbb{Z}^d$, $\varepsilon \ll 1$, be labels for atoms. We consider atomistic deformations $y : \Omega \cap \varepsilon\mathbb{Z}^d \to \mathbb{R}^d$. For fixed $A_0 \in \mathbb{R}^{d\times d}$, $\det A_0 \neq 0$, the macroscopic material domain is $A_0\Omega$ with atomic reference positions $A_0\Omega \cap \varepsilon A_0\mathbb{Z}^d$ and reference configuration $y_{A_0}(x) = A_0 x$.

For a suitable $R_0 > \max\{\max\{|\rho| : \rho \in \mathcal{R}\}, \frac{\sqrt{d}}{4}\}$ (see below), we introduce the following sets of *(semi-)interior* and *boundary atoms*, respectively:

- $\operatorname{sint}_\varepsilon \Omega = \{x \in \Omega \cap \varepsilon\mathbb{Z}^d \colon \operatorname{dist}(x, \partial\Omega) > \varepsilon R_0\}$,
- $\operatorname{int}_\varepsilon \Omega = \{x \in \Omega \cap \varepsilon\mathbb{Z}^d \colon \operatorname{dist}(x, \partial\Omega) > 2\varepsilon R_0\}$,
- $\partial_\varepsilon\Omega = \Omega \cap \varepsilon\mathbb{Z}^d \setminus \operatorname{int}_\varepsilon \Omega$.

We assume that each atom $x \in \varepsilon\mathbb{Z}^d$ only interacts with neighboring atoms belonging to $x+\varepsilon\mathcal{R}$, where the interaction range $\mathcal{R} \subset \mathbb{Z}^d$ is finite (with $\operatorname{span}_\mathbb{Z} = \mathbb{Z}^d$ and $\mathcal{R} = -\mathcal{R}$). For a given atomistic deformation y, such interactions can only depend on the matrix of differences

$$D_{\mathcal{R},\varepsilon} y(x) = \Big(\frac{y(x+\varepsilon\rho) - y(x)}{\varepsilon}\Big)_{\rho\in\mathcal{R}} \qquad (\in \mathbb{R}^{\{1,\dots,d\}\times\mathcal{R}}).$$

For a given body force $f \colon \varepsilon\mathbb{Z}^d \cap \Omega \to \mathbb{R}^d$ and a boundary datum $g \colon \partial_\varepsilon\Omega \to \mathbb{R}^d$, the total energy is assumed to be expressed in terms of a site potential $W_{\rm atom} : (\mathbb{R}^d)^\mathcal{R} \to (-\infty, \infty]$ (independent of ε) satisfying a (mild) symmetry assumption:

$$E_\varepsilon(y; g) = \varepsilon^d \sum_{x\in\operatorname{sint}_\varepsilon \Omega} W_{\rm atom}(D_{\mathcal{R},\varepsilon} y(x)) - \varepsilon^d \sum_{x\in\varepsilon\mathbb{Z}^d\cap\Omega} f(x)\cdot y(x),$$

if $y \in \mathcal{A}_\varepsilon(\Omega, g)$, where the set of admissible deformations is

$$\mathcal{A}_\varepsilon(\Omega, g) = \{y \colon \Omega \cap \varepsilon\mathbb{Z}^d \to \mathbb{R}^d \colon y(x) = g(x) \text{ for all } x \in \partial_\varepsilon\Omega\}.$$

Local minimizers satisfy the equilibrium equations

$$\left\{ \begin{array}{rcll} -\operatorname{div}_{\mathcal{R},\varepsilon}\big(DW_{\rm atom}(D_{\mathcal{R},\varepsilon} y_{\rm atom}(x))\big) & = & f(x) & \text{in } \Omega, \\ y(x) & = & g(x) & \text{on } \partial_\varepsilon\Omega. \end{array} \right.$$

Here for any $M\colon \Omega\cap\varepsilon\mathbb{Z}^d\to\mathbb{R}^{d\times\mathcal{R}}$ we write

$$\operatorname{div}_{\mathcal{R},\varepsilon} M(x)=\sum_{\rho\in\mathcal{R}}\frac{M_\rho(x)-M_\rho(x-\varepsilon\rho)}{\varepsilon}.$$

Link to continuum systems.

The *Cauchy-Born rule* associates to W_{atom} the continuum energy density

$$W_{\mathrm{CB}}(A):=W_{\mathrm{atom}}((A\rho)_{\rho\in\mathcal{R}}).$$

The corresponding continuum boundary value problem reads as

$$\begin{cases} -\operatorname{div}\big(DW_{\mathrm{CB}}(\nabla y(x))\big) &= f(x) \quad \text{in } \Omega,\\ y(x) &= g(x) \quad \text{on } \partial\Omega. \end{cases}$$

Stability.

Linearizing the continuous equation at the affine deformation y_{A_0} and setting $L=D^2W_{\mathrm{CB}}(A_0)\in\mathrm{Bil}(\mathbb{R}^{d\times d})$, since $\operatorname{span}_{\mathbb{R}}\mathcal{R}=\mathbb{R}^d$, the classical *Legendre-Hadamard condition* can be written as

$$\tilde\lambda_{\mathrm{LH}}(L)=\inf_{\xi,\eta\in\mathbb{R}^d\setminus\{0\}}\frac{L[\xi\otimes\eta,\xi\otimes\eta]}{|\xi|^2\sum\limits_{\rho\in\mathcal{R}}(\rho\eta)^2}>0.$$

With $K=D^2W_{\mathrm{atom}}((A_0\rho)_{\rho\in\mathcal{R}})\in\mathrm{Bil}(\mathbb{R}^{\{1,\dots,d\}\times\mathcal{R}})$ and

$$\lambda_\varepsilon(K,\Omega)=\inf_{\substack{y\in\mathcal{A}_\varepsilon(\Omega,0)\\ y\neq0}}\frac{\varepsilon^d\sum\limits_{x\in\operatorname{sint}_\varepsilon\Omega}K[D_{\mathcal{R},\varepsilon}y(x),D_{\mathcal{R},\varepsilon}y(x)]}{\varepsilon^d\sum\limits_{x\in\operatorname{sint}_\varepsilon\Omega}|D_{\mathcal{R},\varepsilon}y(x)|^2}.$$

we consider the *atomistic stability condition*

$$\lambda_{\mathrm{atom}}(K)=\inf_{\varepsilon>0}\lambda_\varepsilon(K,\Omega)=\lim_{\varepsilon\searrow0}\lambda_\varepsilon(K,\Omega)>0,$$

which in fact is independent of Ω (cf. also [7]).

Proposition. *Assume that* $K_{j\rho l\sigma}=K_{l\sigma j\rho}=K_{j(-\rho)l(-\sigma)}$. *Then*

$$\lambda_{\mathrm{atom}}(K)=\inf_{\substack{\xi\in\mathbb{R}^d\setminus\{0\}\\ k\in[0,2\pi)^d\setminus\{0\}}}\frac{K[\xi\otimes c(k),\xi\otimes c(k)]+K[\xi\otimes s(k),\xi\otimes s(k)]}{|\xi|^2(|c(k)|^2+|s(k)|^2)},$$

where $c(k)_\rho=\cos(\rho k)-1$ *and* $s(k)_\rho=\sin(\rho k)$.

Remarks.

(1) The proof with Fourier series techniques is not hard.
(2) We recover the well known fact that $\lambda_{\mathrm{atom}}>0$ (atomistic stability) implies $\lambda_{\mathrm{LH}}>0$ (Legendre-Hadamard condition).
(3) This representation applies directly for models considered in [6, 4].

Solving the continuous equations.

Theorem. *Let $m \in \mathbb{N}_0$, $d < 2m+2$ and let $\Omega \subset \mathbb{R}^d$ be an open, bounded set with C^{m+2}-boundary. Let $r_0 > 0$ and assume that $W_{\rm atom} \in C^{m+3}(\overline{B_{r_0}((A_0\rho)_{\rho\in\mathcal{R}})})$ with $\lambda_{\rm LH}(A_0) > 0$. Then there are $\kappa_1, \kappa_2 > 0$ such that, for $\|g - y_{A_0}\|_{H^{m+2}(\Omega;\mathbb{R}^d)} < \kappa_1$, $\|f\|_{H^m(\Omega;\mathbb{R}^d)} < \kappa_1$, the boundary value problem*

$$\begin{aligned} -\operatorname{div}(DW_{\rm CB}(\nabla y(x))) &= f(x), \qquad \text{if } x \in \Omega, \\ y(x) &= g(x), \qquad \text{if } x \in \partial\Omega, \end{aligned}$$

has exactly one weak solution with $\|y - g\|_{H^{m+2}(\Omega;\mathbb{R}^d)} < \kappa_2$.

Discrete-to-continuum passage.

We introduce the following *discrete (semi-)norms.*

$$\|u\|_{h^1_\varepsilon(\operatorname{sint}_\varepsilon\Omega)} = \Big(\varepsilon^d \sum_{x\in\operatorname{sint}_\varepsilon\Omega} |D_{\mathcal{R},\varepsilon}u(x)|^2\Big)^{\frac12}, \quad \|g\|_{\partial_\varepsilon\Omega,0} = \|T_\varepsilon g\|_{h^1_\varepsilon(\operatorname{sint}_\varepsilon\Omega)},$$

$$\|u\|_{h^{-1}_\varepsilon(\operatorname{int}_\varepsilon\Omega)} = \sup\Big\{\varepsilon^d \sum_{x\in\operatorname{int}_\varepsilon\Omega} u(x)\cdot\varphi(x)\colon \varphi\in\mathcal{A}_\varepsilon(\Omega,0), \|\varphi\|_{h^1_\varepsilon(\operatorname{sint}_\varepsilon\Omega)} = 1\Big\},$$

where $T_\varepsilon g = \operatorname{argmin}\big(\|y\|_{h^1_\varepsilon(\operatorname{sint}_\varepsilon\Omega)}$ subject to $y = g$ on $\partial_\varepsilon\Omega\big)$. We also set $\tilde f(x) = \varepsilon^{-d}\int_{z+(-\frac{\varepsilon}{2},\frac{\varepsilon}{2})^d} f(z)\,dz$ for $x \in z + (-\frac{\varepsilon}{2},\frac{\varepsilon}{2})^d$, $z \in \varepsilon\mathbb{Z}^d$. Let E be an extension operator for all Sobolev spaces, η_ε standard mollifier. If $y \in H^1(\Omega;\mathbb{R}^d)$, write

$$S_\varepsilon y(x) = \eta_\varepsilon * (y_{A_0} + E(y - y_{A_0}))(x) \quad \text{for } x \in \varepsilon\mathbb{Z}^d.$$

Theorem. *Let $d \in \{1,2,3,4\}$ and let $\Omega \subset \mathbb{R}^d$ be an open, bounded set with C^4-boundary. Let $W_{\rm atom} \in C^5(\overline{B_{r_0}((A_0\rho)_{\rho\in\mathcal{R}})})$, $r_0 > 0$, and assume $\lambda_{\rm atom}(A_0) > 0$. There are $K_1, K_2, K_3 > 0$ such that for every $\varepsilon \in (0,1]$, $\gamma \in [\frac{d}{2}, 2]$, $f \in H^2(\Omega;\mathbb{R}^d)$ with $\|f\|_{H^2(\Omega;\mathbb{R}^d)} \le K_1$, $g \in H^4(\Omega;\mathbb{R}^d)$ with $\|g - y_{A_0}\|_{H^4(\Omega;\mathbb{R}^d)} \le K_1$, $f_{\rm atom}\colon \operatorname{int}_\varepsilon\Omega \to \mathbb{R}^d$ with $\|f_{\rm atom} - \tilde f\|_{h^{-1}_\varepsilon(\operatorname{int}_\varepsilon\Omega)} \le K_2\varepsilon^\gamma$, and $g_{\rm atom}\colon \partial_\varepsilon\Omega \to \mathbb{R}^d$ with $\|g_{\rm atom} - S_\varepsilon y\|_{\partial_\varepsilon\Omega,0} \le K_2\varepsilon^\gamma$, (y being the continuous solution to f and g, cf. previous theorem) such that:*

There is a unique $y_{\rm atom} \in \mathcal{A}_\varepsilon(\Omega, g_{\rm atom})$ with $\|y_{\rm atom} - S_\varepsilon y\|_{h^1_\varepsilon(\operatorname{sint}_\varepsilon\Omega)} \le K_3\varepsilon^\gamma$ and

$$-\operatorname{div}_{\mathcal{R},\varepsilon}\big(DW_{\rm atom}(D_{\mathcal{R},\varepsilon}y_{\rm atom}(x))\big) = f_{\rm atom}(x) \qquad \forall\, x \in \operatorname{int}_\varepsilon\Omega.$$

Furthermore, $y_{\rm atom}$ is a strict local minimizer of $E_\varepsilon(\cdot, f_{\rm atom}, g_{\rm atom})$.

Remark. An extension of this result to the dynamic setting, even for long times, has recently been obtained by Braun in [1].

References

[1] J. Braun, *Connecting atomistic and continuous models of elastodynamics*, Arch. Rational Mech. Anal. **224** (2017), 907–953.

[2] J. Braun and B. Schmidt, *On the passage from atomistic systems to nonlinear elasticity theory for general multi-body potentials with p-growth*, Netw. Heterog. Media **8** (2013), 879–912.

[3] J. Braun and B. Schmidt, *Existence and convergence of solutions of the boundary value problem in atomistic and continuum nonlinear elasticity theory*, Calc. Var. Partial Differential Equations **55** (2016), Paper No. 125, 36 pp.
[4] S. Conti, G. Dolzmann, B. Kirchheim, and S. Müller, *Sufficient conditions for the validity of the Cauchy-Born rule close to SO(n)*, J. Eur. Math. Soc. (JEMS) **8** (2006), 515–539.
[5] W. E, P. Ming, *Cauchy-Born rule and the stability of crystalline solids: Static problems*, Arch. Rational Mech. Anal. **183** (2008), 241–297.
[6] G. Friesecke and F. Theil, *Validity and failure of the Cauchy-Born hypothesis in a two-dimensional mass-spring lattice*, J. Nonlinear Sci. **12** (2002), 445–478.
[7] T. Hudson and C. Ortner, *On the stability of Bravais lattices and their Cauchy-Born approximations*, ESAIM:M2AN **46** (2012), 81–110.
[8] C. Ortner and F. Theil, *Justification of the Cauchy-Born approximation of elastodynamics*, Arch. Rational Mech. Anal. **207** (2013), 1025–1073.

On coercivity of boundary integral functionals in high-frequency scattering

Valery Smyshlyaev

Fundamentally, mathematical problems coming from high-frequency scattering often lead to challenges quite similar to those in homogenization and other miltiscale problems, and often require advanced tools of multiscale analysis. One of such problems is that of coercivity of certain quadratic integral functionals associated with combined boundary integral operators in high frequency scattering. The problem originates from numerical analysis, but in its own appears a highly challenging analytical problem.

An obstacle scattering problem is classically stated mathematically as a boundary value problem for Helmholtz equation $\Delta u + k^2 u = 0$ in an unbounded domain $\Omega_+ \subset \mathbb{R}^d$ exterior to a bounded obstacle Ω_-, with say Dirichlet boundary conditions on $\Gamma := \partial\Omega_+$ and Sommerfeld radiation conditions at infinity for (the scattered part of) u. This forms a well-posed problem in appropriate functional spaces with a unique solution.

The above scattering problem in the unbounded domain is often reduced to that on the boundary Γ via classical Green's integral representation. Namely, if $G_k(x,y)$ is the Green's function (fundamental solution) in $\mathbb{R}^d$ ($G = (i/4)H_0^{(1)}(k|x-y|)$ where $H_0^{(1)}$ is Hankel function for $d=2$, and $G = \exp(ik|x-y|)/(4\pi|x-y|)$ for $d=3$), then

$$u(x) \;=\; u^i(x) \;-\; \int_\Gamma G_k(x,y)\frac{\partial u(y)}{\partial n} ds(y), \quad x \in \Omega_+, \tag{1}$$

where u^i is a known incident wave (a solution of the Helmholtz equation in a neighborhood of Ω_-), $u = u^i + u^s$ with u^s denoting the scattered part. Representation (1) allows to reduce the scattering problem to a Boundary Integral Equation (BIE) for $v(x) := \partial u/\partial n$ on Γ in various ways. One is by simply taking a trace of (1) when $x \to \Gamma$, which results in a "single layer" BIE: $S_k v(x) := \int_\Gamma G_k(x,y)v(y)\,ds(y) \;=\; u^i(x) \;=:\; f(x)$. The latter however suffers from loss of uniqueness when k^2 coincides with an eigenvalue λ_j^D of an internal (i.e. in an

unphysical domain Ω_-) Dirichlet problem. An alternative is to take a "Neumann trace", i.e. to differentiate (1) in n and set $x \to \Gamma$. Taking account of "jump conditions", this results in (adjoint) "double layer" BIE:

$$\left(\frac{1}{2}I + D_k'\right) v(x) := \frac{1}{2}v(x) + \int_\Gamma \frac{\partial G_k}{\partial n(x)}(x,y)v(y)\, ds(y) \;=\; \frac{\partial u^i}{\partial n}(x),$$

which in turn suffers from loss of uniqueness when $k^2 = \lambda_j^N$, an interior Neumann eigenvalue.

A way to avoid the loss of uniqueness is by considering a "combined"BIE (CBIE), e.g. a simple (complex) linear combination of single and double-layer BIEs:

$$A_k v \;=\; \left(\frac{1}{2}I + D_k'\right) v \;-\; i\,k\,\eta S_k v \;=\; f = \frac{\partial u^i}{\partial n}(x) \;- i\,\eta k\, u^i(x) \tag{2}$$

with a 'coupling constant' $k\eta$, where $\eta > 0$ ($k \to \infty$). The CBIE (2), due to uniqueness for an associated interior 'impedance' problem (as well as for the exterior Dirichlet problem), is uniquely solvable for all $\eta > 0$ and $k > 0$, and moreover (for Lipschitz Γ) is known to have a bounded inverse A_k^{-1} in $L^2(\Gamma)$.

An extensive literature, see e.g. numerous references in [7], has been devoted to studying properties of A_k and of A_k^{-1}, particularly for large k i.e. at high frequencies. The latter appears to be strongly linked to the notion of *non-trappingness* of the obstacle, i.e. loosely to the absence of closed "billiards" in the exterior Ω_+. For trapping domains, at high frequencies, such closed billiards can support asymptotic "almost eigenmodes": a geometrical optics type almost-solutions to the Helmholtz equation localized near these billiards. (These ideas go back to [1]; see, e.g., [2] and the references therein.)

However for purpose of numerical analysis of Galerkin-type methods for CBIE (2), properties even stronger than the bounds on $\|A_k^{-1}\|$ are required, namely bounds on the *coercivity constant* $\gamma(k) > 0$ (provided such exists):

$$|(A_k\phi, \phi)_{L^2(\Gamma)}| \;\geq\; \gamma(k)\|\phi\|^2_{L^2(\Gamma)}, \quad \forall \phi \in L^2(\Gamma). \tag{3}$$

The reason is that á priori error estimates in Galerkin approximations critically depend, via Lax-Milgram and Cea's lemmas, on $\gamma(k)$, see e.g. [3]–[5] for further details. (Notice that bounds on $\gamma(k)$ imply bounds on $\|A_k^{-1}\|$, but not other way round.)

The above motivates efforts on establishing coercivity for various domains, particularly at high frequencies (for large k). In [3], coercivity with $\gamma = 1/2$ for $\eta = 1$ and k sufficiently large was proved for a circle or a sphere using Fourier analysis. In [4] it was proved for Lipschitz star-shaped domains for all k with a constant γ independent of k, but for a particularly modified CBIE (the so-called "star-combined" BIE). Finally, in [5] coercivity for a classical CBIE (2) was proved for uniformly convex smooth scatterers with γ arbitrarily close to $1/2$ for large enough k and η. The results in [4] and [5] used some non-trivial modifications of "Morawetz multipliers", e.g. [6].

It is reasonable to expect that, for high frequencies, the coercivity property depends on some form of non-trappingness. Recent work [7], see Remark 6.6, provides an example of loss of a uniform in k coercivity for some classically non-trapping domains (which could however still be viewed as trapping in certain generalized sense). Remaining open question is whether coercivity still holds, possibly with $\gamma(k)$ mildly degenerating as $k \to \infty$, for "strongly non-trapping" (non-convex) domains like e.g. smooth star-shaped ones.

Namely, for a wide class of non-trapping domains, one might hope to prove that for certain $\gamma_0 > 0$ and possibly also $\alpha > 0$ there exists $\gamma > 0$, such that for any $v_k \in L^2(\Gamma)$, $\|v_k\|_{L^2} = 1$,

$$\liminf_{k\to\infty} |(A_k v_k, v_k)| \geq \gamma_0 \, k^{-\alpha}.$$

One can hope to exploit the fact that, asymptotically for large k, in the quadratic functional

$$(Kv_k, v_k) = (Dv_k - i\eta S_k v_k, v_k) = \int_\Gamma \int_\Gamma K(x,y) v_k(x) \overline{v_k(y)} dS(x) dS(y),$$

with oscillatory (compact) kernel $K(x,y)$, the small "elements" $v_k(x)dS(x)$ and $v_k(y)dS(y)$ interact only through "billiard-related" frequencies in v_k near x and y. This may naturally suggest that certain tools from multi-scale analysis, such as e.g. Wigner or $H-$measures, might be relevant. For example, let $v_k \in L^2(\Gamma)$ and $\|v_k\|_{L^2} = 1$. Then, up to a subsequence $k_n \to \infty$, v_{k_n} appropriately (weakly) converges to a "two-scale" $v(x, kx)$, where $v(x,z)$ has a Fourier transform $\hat{v}(x,\xi)$ in "fast variable" z. Then one can hope that, asymptotically as $k \to \infty$, the functional $I_k(v_k) := (Kv_k, v_k)$ behaves like a "two-scale" limit functional $I_\infty(\hat{v}(x,\xi))$. The latter might account explicitly for the billiard-type interactions only, which for non-trapping domains (i.e. in the absence of closed billiards) in turn might maintain certain coercivity properties by a direct inspection. Realization of such a program would probably require establishing appropriate version of a key (two-scale) compactness property, for justifying such a limit passage.

References

[1] J.B. Keller and S.I. Rubinow, *Asymptotic solution of eigenvalue problems*, Ann. Phys. **9** (1960), 24–75.

[2] V.M. Babich and V.S. Buldyrev, *Asymptotic Methods in Short-Wavelength Diffraction Theory*, Alpha Science Series on Wave Phenomena, 2008.

[3] V. Domínguez, I.G. Graham, and V.P. Smyshlyaev, *A hybrid numerical-asymptotic boundary integral method for high-frequency acoustic scattering*, Numer. Math. **106** (2007), 471–510.

[4] E.A. Spence, S.N. Chandler-Wilde, I.G. Graham, and V.P. Smyshlyaev, *A new frequency-uniform coercive boundary integral equation for acoustic scattering*, Comm. Pure Appl. Math. **64** (2011), 1384–1415.

[5] E.A. Spence, I.V. Kamotski, and V.P. Smyshlyaev, *Coercivity of combined boundary integral equations in high frequency scattering*, Comm. Pure Appl. Math. **68** (2015), 1587–1639.

[6] C.S. Morawetz and D. Ludwig, *An inequality for the reduced wave operator and the justification of geometrical optics*, Comm. Pure Appl. Math. **21** (1968), 187–203.
[7] S.N. Chandler-Wilde, E.A. Spence, A. Gibbs, and V. P. Smyshlyaev, *High-frequency bounds for the Helmholtz equation under parabolic trapping and applications in numerical analysis*, submitted. arXiv:1708.08415.

Carbon nanotubes from the molecular-mechanical viewpoint

Ulisse Stefanelli

Carbon nanotubes are long, hollow structures showing cylindrical symmetry [2]. Their walls consist of a single (or multiple) one-atom-thick layer of carbon atoms arranged in a hexagonal pattern. Such a specific structure is responsible for the remarkable properties of these materials in terms of strength, electric and thermal conductivity, chemical sensitivity, transparency, and light weight. One can visualize a carbon nanotube as the result of rolling up a patch of a regular hexagonal lattice. Depending on the different possible realizations of this rolling-up, different topologies may arise, giving rise to *zigzag, armchair*, and *chiral* nanotubes. These topologies are believed to have a specific impact on the mechanical and electronic properties of the nanotube, which can go from being highly conducting to semiconducting.

A variety of models for carbon nanotubes has been set forth, ranging from purely geometrical descriptions [1, 2] to continuum-mechanical models as rods, shells, or even solids. Our interest is in modeling such structures within the frame of Molecular Mechanics: We identify carbon nanotubes with point configurations $\{x_1, \dots, x_n\} \in \mathbb{R}^{3n}$ corresponding to atomic positions. The atoms are interacting via a *configurational energy* $E = E(x_1, \dots, x_n)$ given in terms of classical potentials and taking into account both attractive-repulsive *two-body* interactions, minimized at a certain bond length, and *three-body* terms favoring specific angles between bonds [8]. Specifically, we define

$$E(\{x_1, \dots, x_n\}) = \frac{1}{2} \sum_{\mathrm{NN}} v_2(|x_i - x_j|_L) + \frac{1}{2} \sum_{\mathrm{NN}} v_3(\alpha_{ijk}). \tag{1}$$

Here, $v_2 : \mathbb{R}^+ \to [-1, \infty)$ is a smooth *two-body potential* attaining its minimal value only at 1 with $v_2(1) = -1$ with $v_2''(1) > 0$ and vanishing shortly after 1 and the corresponding sum is taken on nearest neighbors (NN) only. The distance $|x_i - x_j|_L$ is taken modulo L-periodicity in a fixed direction, representing indeed the axis of the nanotube. The angle α_{ijk} is determined (up to complementarity) by the segments $x_j - x_i$ and $x_k - x_j$ where $\{x_i, x_j\}$ and $\{x_k, x_j\}$ are nearest neighbors. The *three-body potential* $v_3 : [0, 2\pi] \to [0, \infty)$ is smooth and symmetric around π with minimum value 0 just at $2\pi/3$ and $4\pi/3$ and with $v_3''(2\pi/3) > 0$. These choices describe, although to a schematic extent, the phenomenology of sp^2-covalent bonding in carbon, i.e., the bonding model in carbon nanotubes.

Carbon nanotubes are identified with extremizers of the configurational energy, namely by solving $\nabla E = 0$ in $\mathbb{R}^{3n}$ with very large n. The complexity of such a description can be tamed by restricting to specific subclasses of *objective* [4], highly

symmetric configurations. In the *zigzag* topology, these can be seen as orbits of two atoms a under the action of a prescribed isometry group generated by a translation combined with a rotation along the axis and by a simple translation. In other words, all atoms of an objective nanotube see the same local geometry, which is in turn completely determined by a small set of scalars (angles and bond lengths). Correspondingly, the energy of such objective configurations $E_{\rm obj}$ is defined on a subset of $\mathbb{R}^m$ for m small. Extremizers of such $E_{\rm obj}$, i.e. carbon nanotubes which minimize energy *within the class* of objective nanotubes, can be easily determined. Such an optimal objective nanotube geometry is new. In particular, it does not correspond to the geometric models [1, 2] available.

The question is now how well the optimal objective nanotube describes extremizers of E and how is this approach influenced by mechanics. One can in fact apply a stretching on configurations by simply modifying the period L in the definition of the energy. We have analyzed these issues in [3, 5, 6] where we prove the following facts:

(a) The optimal objective nanotube C^* is a strict local minimizer of E, namely $E(C) > E(C^*)$ for all nontrivial and possibly nonobjective small perturbations of C^*.

(b) By imposing a small *stretching* $L + \delta L$, one still finds a unique optimal objective nanotube. This is strictly locally minimizing $E_{L+\delta L}$ among all close $(L + \delta L)$-periodic possibly nonobjective configurations.

Note that item (b) proves the so-called Cauchy-Born rule in this setting. As a matter of illustration of (a)-(b), the result of a Monte Carlo simulation for random perturbations and different stretchings is reported in Figure 1 below.

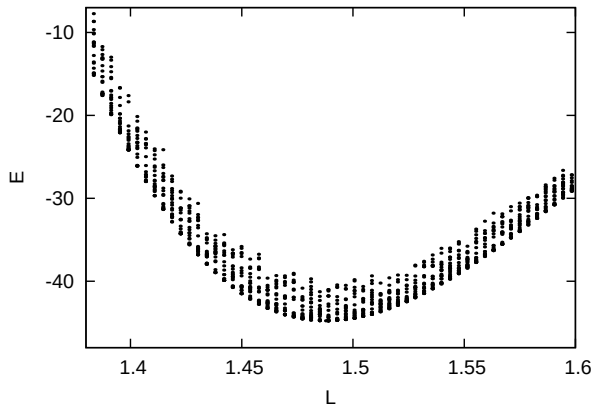

FIGURE 1. Monte Carlo simulation.

For each given L, the lowermost dot in the Figure 1 is the energy of the optimal objective configuration and those above it correspond to the energy of random, nonobjective perturbations. The lower envelope of the cloud in Figure 1 is the elastic energy of the nanotube as a function of its stretching. A discussion on the stability for other carbon structures including carbyne, graphene, fullerenes, and diamond can be found in [7].

References

[1] B. J. Cox, J. M. Hill. Exact and approximate geometric parameters for carbon nanotubes incorporating curvature, *Carbon*, 45 (2007), 1453–1462.

[2] M. S. Dresselhaus, G. Dresselhaus, R. Saito. Carbon fibers based on C_{60} ad their symmetry, *Phys. Rev. B*, 45 (1992), 11:6234–6242.

[3] M. Friedrich, E. Mainini, P. Piovano, U. Stefanelli. Characterization of optimal carbon nanotubes under stretching and validation of the Cauchy-Born rule. Submitted, 2017. Preprint at `arXiv:1706.01494`.

[4] R. D. James. Objective structures, *J. Mech. Phys. Solids*, 54 (2006), 2354–2390.

[5] E. Mainini, H. Murakawa, P. Piovano, U. Stefanelli. Carbon-nanotube geometries: analytical and numerical results, *Discrete Contin. Dyn. Syst. Ser. S*, 10 (2017), 141–160.

[6] E. Mainini, H. Murakawa, P. Piovano, U. Stefanelli. Carbon-nanotube geometries as optimal configurations. Submitted, 2016.

[7] U. Stefanelli. Stable carbon configurations, *Boll. Unione Mat. Ital (9)*, to appear, 2017.

[8] J. Tersoff. New empirical approach for the structure and energy of covalent systems. *Phys. Rev. B*, 37 (1988), 6991–7000.

Solitary waves in nonintegrable lattices

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(joint work with L. Truskinovsky, J. Cuevas-Maraver, P. G. Kevrekidis, H. Xu)

The interplay between dispersion and nonlinearity in many physical systems leads to the formation of solitary traveling waves, localized coherent structures that carry energy through the system. For example, such waves were experimentally observed in granular materials [1] and are believed to be responsible for energy transport in muscle proteins [2]. Much of the interest in these nonlinear waves was triggered by the pioneering study [3] of the Fermi-Pasta-Ulam (FPU) problem, which can be written in the rescaled form

$$\ddot{w}_n = f(w_{n+1}) - 2f(w_n) + f(w_{n-1}). \tag{1}$$

Here w_n is the strain associated with the relative motion of the nth and $(n-1)$th masses in a one-dimensional chain, and $f(w)$ is a nonlinear nearest-neighbor interaction force. The subsequent work [4] has revolutionized the nonlinear science by connecting the FPU problem to the Korteweg-de Vries (KdV) equation that describes its low-energy quasicontinuum limit and showing that the near-recurrence of the initial data observed in [3] in this limit can be attributed to formation and interactions of solitary waves. Such waves have the form $w_n(t) = w(x)$, $x = n - Vt$, where V is the velocity of the wave, and tend to a constant (typically zero) at infinity. In integrable systems solitary waves, known as solitons, are now well understood, with one-dimensional Toda lattice [5] being the most prominent example that has an exact solution covering a broad range of behaviors from delocalized low-energy waves in the KdV limit to highly localized high-energy waves. Most discrete systems, however, are nonintegrable. In this case understanding the transition from the KdV limit to the strongly discrete waves has mostly relied on numerical [6] and quasicontinuum [7] approximations.

In recent work [8] we constructed a nonintegrable analog of the Toda family of solitons for the FPU problem (1) with a piecewise linear continuous $f(w)$:

$$f(w) = w, \quad w \le w_c, \qquad f(w) = \alpha(w - w_c) + w_c, \quad w \ge w_c, \tag{2}$$

where $\alpha > 1$ and $w_c > 0$. The obtained exact infinite series solution captures the entire crossover velocity range between the low-energy limit and strongly localized waves that involve only one particle moving at a time. Truncation of the series solution involving progressively smaller characteristic wavelengths produces a nested set of approximate solutions. Even the simplest solution of this type that accounts only for the longest wavelengths provides a better overall approximation of solitary waves than some conventional quasicontinuum models.

Numerical simulations [8, 9] suggest stability of the constructed solutions for velocities above a certain threshold, where the system's energy, $\mathcal{H}$, increases with the velocity V of the solitary wave, and instability for supersonic velocities below the threshold, where $d\mathcal{H}/dV < 0$. The instability near the sonic limit is an artifact of the piecewise linear form of (2), as demonstrated in [10], where the problem with a smoothened $f(w)$ is investigated both numerically and by analyzing the spectrum of the associated linear operator. In this case, the instability occurs in a narrow velocity interval with the lower bound strictly above the sonic limit.

The analysis is extended [11] to the case including harmonic second-neighbor interactions of relative strength measured by the parameter β, with the governing equations

$$\ddot{w}_n = f(w_{n+1}) - 2f(w_n) + f(w_{n-1}) + \frac{\beta}{4}(w_{n+2} - 2w_n + w_{n-2}), \tag{3}$$

where $\beta > -1$ is assumed to ensure stability of the homogeneous deformation. We show that when the interactions are strongly competitive, with $-1 < \beta < -1/4$, the waves must be *strictly supersonic*, in the sense that solitary wave solutions do not exist in a velocity gap above the sonic limit $c = \sqrt{1+\beta}$ and below a certain β-dependent velocity bound. Solutions with velocities just above the bound have the form of slowly modulated oscillations. In contrast, there is no such gap for $\beta \ge -1/4$, and the near-sonic solutions have a monotone decay at infinity [12].

Construction of planar solitary waves $w_{l,m}(t) = w(x)$, $x = l\cos\phi + m\sin\phi - Vt$, for the two-dimensional square lattice problem

$$\ddot{w}_{l,m} = f(w_{l+1,m}) + f(w_{l-1,m}) + f(w_{l,m+1}) + f(w_{l,m-1}) - 4f(w_{l,m}) \tag{4}$$

with $f(w)$ given by (2) reveals a strong anisotropy in the dependence of the width and height of the wave on the angle ϕ of propagation that is well captured by truncated solutions including sufficiently short wavelengths [13].

References

[1] C. Coste, E. Falcon, and S. Fauve, *Solitary waves in a chain of beads under Hertz contact*, Phys. Rev. E **56** (1997), 6104–6117.
[2] D. Hochstrasser, F. G. Mertens, and H. Büttner, *Energy transport by lattice solitons in α-helical proteins*, Phys. Rev. A **40** (1989), 2602–2610.
[3] E. Fermi, J. Pasta, and S. Ulam, *Studies of nonlinear problems*, Tech. Rep. LA-1940, Los Alamos Scientific Laboratory (1955).
[4] N. J. Zabusky and M. D. Kruskal, *Interaction of "solitons" in a collisionless plasma and the recurrence of initial states*, Phys. Rev. Lett. **15** (1965), 240–243.
[5] M. Toda, *Theory of nonlinear lattices*, Springer-Verlag (1981).
[6] J. C. Eilbeck and R. Flesch, *Calculation of families of solitary waves on discrete lattices*, Phys. Lett. A **149** (1990), 200–202.
[7] J. A. D. Wattis, *Approximations to solitary waves on lattices, II: Quasicontinuum methods for fast and slow waves*, J. Phys. A **26** (1993), 1193–1209.
[8] L. Truskinovsky and A. Vainchtein, *Solitary waves in a nonintegrable Fermi-Pasta-Ulam chain*, Phys. Rev. E **90** (2014), 042903.
[9] J. Cuevas-Maraver, P. G. Kevrekidis, A. Vainchtein, and H. Xu, *A unifying perspective: solitary traveling waves as discrete breathers in Hamiltonian lattices and energy criteria for their stability*, submitted, arXiv preprint arXiv:1701.04882 (2017).
[10] H. Xu, J. Cuevas-Maraver, P. G. Kevrekidis, and A. Vainchtein, *An energy-based stability criterion for solitary traveling waves in Hamiltonian lattices*, submitted (2017).
[11] L. Truskinovsky and A. Vainchtein, *Strictly supersonic solitary waves in lattices with competing interactions*, in preparation (2017).
[12] J. A. D. Wattis, *Approximations to solitary waves on lattices, III: the monatomic lattice with second-neighbour interactions*, J. Phys. A **29** (1996), 8139–8157.
[13] A. Vainchtein. *Solitary wave propagation in a two-dimensional lattice*, in preparation (2017).

Nonlinear and Linear Elastodynamics Transformation Cloaking

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(joint work with Ashkan Golgoon)

We formulate the problem of elastodynamics transformation cloaking in both nonlinear and linear elastodynamics. In particular, it is noted that a cloaking transformation is neither a spatial nor a referential change of frame (coordinates); a cloaking transformation maps the boundary-value problem of an isotropic and homogeneous elastic body (virtual problem) to that of an anisotropic and inhomogeneous elastic body with a hole reinforced by a cloak that is to be designed (physical problem). The virtual body has a desired mechanical response while the physical body is designed to mimic the same response outside the cloak using a cloaking transformation. We determine the constitutive equations of nonlinear elastic cloaks and the elastic constants of linear elastic cloaks. It is shown that the elastic constants of a linear elastic cloak are fully symmetric. Finally, we present an example of a linear elastic cloak.

Stochastic homogenisation of free-discontinuity functionals

Caterina Ida Zeppieri
(joint work with Filippo Cagnetti, Gianni Dal Maso, Lucia Scardia)

In the Calculus of Variations the terminology free-discontinuity functionals usually refers to those functionals with competing volume and surface terms. A typical example is that of an integral functional of the form

$$E(u) = \int_A f(x, \nabla u)\, dx + \int_{S_u \cap A} g(x, [u], \nu_u)\, d\mathcal{H}^{n-1}, \tag{1}$$

depending on both $u\colon A \subset \mathbb{R}^n \to \mathbb{R}^m$ and on its discontinuity set S_u, whose shape and location are not known *a priori*. The natural functional setting for E is that of special functions of bounded variation $SBV(A, \mathbb{R}^m)$. Then ∇u denotes the approximate differential of u, $[u]$ stands for the difference $u^+ - u^-$ between the approximate limits of u on both sides of the discontinuity set S_u, and ν_u denotes the (generalised) normal to S_u.

In the last decades the mathematical theory of free-discontinuity problems had a great development and its manifold applications range from Computer Vision to Materials Science. In typical applications one has to deal with families of functionals of type (1); *i.e.,* functionals depending on some small positive parameter ε, whose nature depends on the specific problem under consideration, and try to establish some emergent properties in the limit of $\varepsilon \to 0$. Further, in many relevant applications (such as *e.g.* the study of composite materials) the integrands f and g may also vary according to some (spatial) periodicity, or more generally to some random law. One is then led to consider families of functionals of the form

$$E_\varepsilon(\omega)(u) = \int_A f\left(\omega, \frac{x}{\varepsilon}, \nabla u\right)\, dx + \int_{S_u \cap A} g\left(\omega, \frac{x}{\varepsilon}, [u], \nu_u\right)\, d\mathcal{H}^{n-1}, \tag{2}$$

where ω belongs to the sample space Ω of a probability space $(\Omega, \mathcal{T}, P)$ and labels the realisations of the integrands f and g, which are now understood as random variables.

When f and g do not depend on ω and are periodic in the spatial variable the limit behaviour of E_ε can be determined appealing to the classical homogenisation theory [3]. The latter asserts that, under standard growth and coercivity conditions (and mild regularity assumptions) on f and g the deterministic functionals E_ε behave macroscopically like a homogeneous free-discontinuity functional. Further, in the homogenisation process there is no interaction between volume and surface energy.

In this talk we discuss the asymptotic behaviour of free-discontinuity functionals as in (2) where the integrands f and g are random variables and their realisations satisfy the following assumptions. We fix six constants $p, c_1, \dots, c_5$, with $1 < p < +\infty$, $0 < c_1 \le c_2 < +\infty$, $1 \le c_3 < +\infty$, and $0 < c_4 \le c_5 < +\infty$, and two nondecreasing continuous functions σ_1, $\sigma_2\colon [0, +\infty) \to [0, +\infty)$ such that $\sigma_1(0) = \sigma_2(0) = 0$.

The volume integrand $f\colon \mathbb{R}^n \times \mathbb{R}^{m\times n} \to [0, +\infty)$ has to satisfy:

($f1$) (measurability) f is Borel measurable on $\mathbb{R}^n \times \mathbb{R}^{m\times n}$;
($f2$) (continuity in ξ) for every $x \in \mathbb{R}^n$ we have

$$|f(x,\xi_1) - f(x,\xi_2)| \le \sigma_1(|\xi_1 - \xi_2|)\big(1 + f(x,\xi_1) + f(x,\xi_2)\big)$$

for every ξ_1, $\xi_2 \in \mathbb{R}^{m\times n}$;
($f3$) (bounds) for every $x \in \mathbb{R}^n$ and every $\xi \in \mathbb{R}^{m\times n}$

$$c_1|\xi|^p \le f(x,\xi) \le c_2(1 + |\xi|^p).$$

The surface integrand $g\colon \mathbb{R}^n \times \mathbb{R}^m_0 \times \mathbb{S}^{n-1} \to [0,+\infty)$ satisfies:
($g1$) (measurability) g is Borel measurable on $\mathbb{R}^n \times \mathbb{R}^m_0 \times \mathbb{S}^{n-1}$;
($g2$) (continuity in ζ) for every $x \in \mathbb{R}^n$ and every $\nu \in \mathbb{S}^{n-1}$ we have

$$|g(x,\zeta_2,\nu) - g(x,\zeta_1,\nu)| \le \sigma_2(|\zeta_1 - \zeta_2|)\big(g(x,\zeta_1,\nu) + g(x,\zeta_2,\nu)\big)$$

for every ζ_1, $\zeta_2 \in \mathbb{R}^m_0$;
($g3$) (estimate for $|\zeta_1| \le |\zeta_2|$) for every $x \in \mathbb{R}^n$ and every $\nu \in \mathbb{S}^{n-1}$ we have

$$g(x,\zeta_1,\nu) \le c_3\, g(x,\zeta_2,\nu)$$

for every ζ_1, $\zeta_2 \in \mathbb{R}^m_0$ with $|\zeta_1| \le |\zeta_2|$;
($g4$) (estimate for $c_3|\zeta_1| \le |\zeta_2|$) for every $x \in \mathbb{R}^n$ and every $\nu \in \mathbb{S}^{n-1}$ we have

$$g(x,\zeta_1,\nu) \le\ g(x,\zeta_2,\nu)$$

for every ζ_1, $\zeta_2 \in \mathbb{R}^m_0$ with $c_3|\zeta_1| \le |\zeta_2|$;
($g5$) (bounds) for every $x \in \mathbb{R}^n$, $\zeta \in \mathbb{R}^m_0$, and $\nu \in \mathbb{S}^{n-1}$

$$c_4 \le g(x,\zeta,\nu) \le c_5(1 + |\zeta|);$$

($g6$) (symmetry) for every $x \in \mathbb{R}^n$, $\zeta \in \mathbb{R}^m_0$, and $\nu \in \mathbb{S}^{n-1}$

$$g(x,\zeta,\nu) = g(x,-\zeta,-\nu).$$

The random environment is then described by a group of P-preserving transformations $(\tau_z)_{z\in\mathbb{Z}^n}$ defined on the probability space $(\Omega,\mathcal{T},P)$.

For homogenisation to occur we consider only those randomness having some kind of self-repeating structure. This property can be quantified in terms of $(\tau_z)_{z\in\mathbb{Z}^n}$ by requiring that f and g are stationary; *i.e.,* for every $z \in \mathbb{Z}^n$ and P-almost surely

$$f(\omega, x+z, \xi) = f(\tau_z\omega, x, \xi) \quad \forall (x,\xi) \in \mathbb{R}^n \times \mathbb{R}^{m\times n}, \tag{3}$$

$$g(\omega, x+z, \zeta, \nu) = g(\tau_z\omega, x, \zeta, \nu) \quad \forall (x,\zeta,\nu) \in \mathbb{R}^n \times \mathbb{R}^m_0 \times S^{n-1}. \tag{4}$$

The two conditions as above ensure that the statistical properties of the medium are invariant under translations; this will allow us to reconstruct, in a suitable statistical sense, the overall limit behaviour of E_ε by the knowledge of its local behaviour on a sequence of increasingly larger "fundamental cells".

To analyse the limit of E_ε we first regard ω as a fixed parameter and study the limit behaviour of the deterministic (and in general non periodic) functionals $E_\varepsilon(\omega)$. The convergence of functionals of type $E_\varepsilon(\omega)$ has been recently studied in [5] where, among other, the homogenisation of free-discontinuity functionals without periodicity assumptions has been addressed. Specifically, [5, Theorem

3.8] provides us with a sufficient condition for the Γ-convergence of the family $\big(E_\varepsilon(\omega)\big)_\varepsilon$ towards a homogeneous free-discontinuity functional of the form

$$E_{\rm hom}(\omega)(u) := \int_A f_{\rm hom}\left(\omega, \nabla u\right)\, dx + \int_{S_u\cap A} g_{\rm hom}\left(\omega, [u], \nu_u\right)\, d\mathcal{H}^{n-1},$$

for suitable Borel functions $f_{\rm hom}(\omega,\cdot)$ and $g_{\rm hom}(\omega,\cdot,\cdot)$. The aforementioned sufficient condition amounts to the existence and independence of x of the two following limits

$$\lim_{r\to 0^+}\frac{1}{r^n}\inf\int_{Q_r(rx)} f(\omega, y, \nabla u(y))dy =: f_{\rm hom}(\omega,\xi), \tag{5}$$

and

$$\lim_{r\to 0^+}\frac{1}{r^{n-1}}\inf\int_{S_u\cap Q^\nu_r(rx)} g(\omega, y, [u](y), \nu_u(y))d\mathcal{H}^{n-1}(y) =: g_{\rm hom}(\omega,\zeta,\nu) \tag{6}$$

where the infimum in (5) is taken among functions in $W^{1,p}(Q_r(rx),\mathbb{R}^m)$ satisfying $u(y)=\xi y$ near $\partial Q_r(rx)$, while the infimum in (6) is taken among all functions u in $SBV(Q^\nu_r(rx),\mathbb{R}^m)$ satisfying $\nabla u = 0$ $\mathcal{L}^n$-a.e. in $Q^\nu_r(rx)$ and

$$u(y) = u_{rx,\zeta,\nu}(y) := \begin{cases}\zeta & \text{if } (y-rx)\cdot\nu \geq 0\\ 0 & \text{if } (y-rx)\cdot\nu < 0\end{cases} \qquad \text{near } \partial Q^\nu_r(rx).$$

Then in a second (stochastic) step we show that the sufficient condition as above is fulfilled *almost surely*; *i.e.,* the two limits in (5) and (6) exist for P-a.e. $\omega\in\Omega$. As for the case of stochastic homogenisation of volume functionals [6] this step heavily relies on the stationarity assumption on f and g. Specifically, the almost sure existence of the limit in (5) follows as in [6] by first proving that, for every fixed $\xi\in\mathbb{R}^{m\times n}$, the map

$$(\omega, A)\mapsto \inf\left\{\int_A f(\omega, y, \nabla u(y))dy\colon u\in W^{1,p}(A,\mathbb{R}^m),\ u(y)=\xi y \text{ near } \partial A\right\}$$

defines a *subadditive stochastic process* on $\Omega\times\mathcal{I}_n$ (where $\mathcal{I}_n$ denotes the class of n-dimensional intervals) and then invoking the pointwise subadditive Ergodic Theorem of Ackcoglou and Krengel [1]. Though the proof of the existence of the limit in (6) follows a similar strategy as for the volume case, the analysis of surface random functionals is particularly delicate and requires some additional care. Indeed, two main differences between volume and surface energies are immediately apparent from (6). Namely, the latter shows a "mismatch" between the surface scaling r^{n-1} and the minimisation problem

$$\inf\left\{\int_{S_u\cap Q^\nu_r(rx)} g(\omega, y, [u], \nu_u)d\mathcal{H}^{n-1}\colon u\in SBV(Q^\nu_r(rx),\mathbb{R}^m),\right. \tag{7}$$
$$\left.\nabla u = 0, \text{ a.e. in } Q^\nu_r(rx),\ u = u_{rx,\zeta,\nu} \text{ on } \partial Q^\nu_r(rx)\right\}$$

which is defined on the n-dimensional cube $Q_r^\nu(rx)$. Moreover, the explicit dependence of the boundary datum $u_{rx,\zeta,\nu}$ on the spacial variable x results into an additional difficulty in the proof of (6). Then, similarly as in [2], we first set $x = 0$ in (7) and then provide a systematic way to associate to (7) a map defined on $\Omega \times \mathcal{I}_{n-1}$ ($\mathcal{I}_{n-1}$ being the class $(n-1)$-dimensional intervals). This map then turns out to be the sought for $(n-1)$-dimensional subadditive stochastic process, the main difficulty being here the proof of the measurability of the process.

As a final step we show that the choice $x = 0$ is not "special"; *i.e.,* that the limit in (6) actually defines a homogeneous random surface-integrand $g_{\hom}$. This is done appealing to the Birkhoff's Ergodic Theorem in the spirit of [4], where a similar issue is solved by proving the translation invariance of a first passage percolation formula.

Finally, if f and g are ergodic (*i.e.,* they satisfy (3) and (4) for $(\tau_z)_{z\in\mathbb{Z}^n}$ ergodic) the homogenisation becomes effective and the functional $E_{\hom}$ is deterministic.

References

[1] M. A. Akcoglu and U. Krengel, *Ergodic theorems for superadditive processes*, J. reine angew. Math. **323** (1981), 53–67.

[2] R. Alicandro, M. Cicalese, and M. Ruf, *Domain formation in magnetic polymer composites: an approach via stochastic homogenization*, Arch. Rat. Mech. Anal. **218** (2015), 945–984.

[3] A. Braides, A. Defranceschi, and E. Vitali, *Homogenization of Free Discontinuity Problems*, Arch. Ration. Mech. Anal. **135** (1996), 297–356.

[4] A. Braides, A. Piatnitski, *Homogenization of surface and length energies for spin systems*, J. Funct. Anal. **264**, 1296–1328 (2013).

[5] F. Cagnetti, G. Dal Maso, L. Scardia, and C. I. Zeppieri, Γ-*convergence of free-discontinuity problems*, submitted. Available at http://cvgmt.sns.it/paper/3371/.

[6] G. Dal Maso and L. Modica, *Nonlinear stochastic homogenization and ergodic theory*, J. reine angew. Math., **368** (1986), 28–42.

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