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Review of “An energy approach to asymptotic, higher-order, linear homogenization”

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^E Editor

Review of version 2

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Note that version 2 was uploaded soon after version 1 to fix small issues identified by the authors.

Authors

We thank all four reviewers very much for their careful reading of our manuscript and for their insightful comments.

Reviewer 1 (Pierre SEPPECHER)

In the manuscript entitled “An energy approach to asymptotic, higher-order, linear homogenization” the authors, B. Audoly and C. Lestringant, propose a generic method for computing the effective properties of micro-structured elastic materials with a special focus on discrete systems. They use a method based on the asymptotic study of the elastic energy. Indeed this method brings significant benefits. In particular, it allows to take into account boundary conditions. The authors highlight this fact but do not illustrate it.

The methods rely on the fact that the effective energy comes from the partial minimization of the starting energy : this is due to the fact that, for a given macroscopic strain, the material adopt the least energetic configuration at the microscopic level. This well-known fact is the base of the so-called “cell problem” in classical homogenization.

The authors propose a generic version of this partial minimization pushing it to higher order homogenization. They even offer an open-source symbolic Mathematica library for doing it. I have not tested it, but I think it may be very useful for studying different geometries and material properties while avoiding painful computations. For this reason I think that the paper deserves publication.

Reviewer

A similar algebraic generic procedure for homogenizing discrete structure has been proposed in [AS18b] (Houssam Abdoul-Anzizand and Pierre Seppecher. Mathematics and mechanics of complex systems, 6(3):213–250, 2018). It would be pertinent to compare the two methods. Do they give similar or different results on some specific examples?

Authors

Following this suggestion, we have added a new illustration example in §4.3 (frame truss homogenized into a Timoshenko beam) and have checked that the results are consistent with [AS18b]. This example is indeed an interesting addition as it illustrates how the homogenization procedure can be tailored by changing the definition of the macroscopic variables l .

Reviewer However, the manuscript skips several difficulties. It is frankly but lightly written (in Remark 2) that “definitions of the macroscopic strain and the microscopic degrees of freedom will not be provided”. And a bit earlier that “The task of casting a given problem into the generic form proposed in this section is not particularly difficult but has to be carried out on a case-by-case basis.” Determining which type of model best describes the effective behavior is not easier than computing the parameters of the chosen model. This is well illustrated by the proposed example (Section 4) where, for setting up the input of the homogenization procedure, the authors need to use “the classical theory for linear, planar beams” where “the two relevant strain measures are the stretching strain and the bending strain”. They “thus anticipate that the homogenized energy will depend on them”. How can their method ensure that a Timoshenko model is not a more appropriate model for describing the considered beam?

Authors When set up appropriately, our approach is capable of generating a Timoshenko model, see the new Section 4.3. Comparing the respective merits of different models is beyond the scope of our manuscript, which is focused on carrying homogenization for a specific assignment of macroscopic vs. microscopic strain (\mathbf{l}, \mathbf{y}) . This assignment reflects scaling assumptions that are used on input in the literature on homogenization.

Reviewer There is a global inconstancy (an inconstancy shared by very many papers dealing with higher order homogenization) in the asymptotic procedure leading to higher gradient energies. As said by the authors “One of the key assumptions of homogenization is that there is a separation of scales between a microscopic length (typically the spatial period of the underlying discrete lattice or periodic continuum) and the size of the domain” and “the goal of homogenization is to deliver an effective model applicable at the macroscopic scale, by hiding the details taking place at the microscopic scale.” The higher order macroscopic model obtained in (11) contains corrective terms which are active only when variations occur at the microscopic scale (this is not so easy to see because of the implicit presence of the small parameter as mentioned in Remark 6). Can one say to be hiding details taking place at the microscopic scale while finally taking them into account in the effective energy?

Authors The answer is a frank ‘yes’. We do hide the detailed microscopic solution (\mathbf{y}) in the homogenized model, while accounting for it accurately. We do not see any contradiction between ‘hiding’ (we eliminate the quantity \mathbf{y} , by solving an elastic problem) and ‘taking it into account’—in fact, doing so is precisely the point of homogenization. Dimension reduction does the same, by hiding the details of deformation in the cross-sections, while resolving them accurately under the hood and delivering an effective energy that accounts for them.

Note: we are assuming that the reviewers means *inconsistency* rather than *inconstancy*.

Reviewer This inconstancy may have heavy consequences. The example of Section 4 enlightens that. The effective energy obtained there is not positive: it cannot be a good approximation of the starting positive energy. The authors are aware of this fact that they describe as “an undesirable property of higher-order gradient models that has been documented by several authors for various elastic structures” which “calls for a regularization of the functional”.

Authors We disagree with this statement. Consider the following identity (integration by parts):

$$\psi_1 = \psi_2 + \delta,$$

where

$$\begin{aligned}\psi_1 &= \int_a^b \frac{1}{2} (\varepsilon + \varepsilon'')^2 dx \\ \psi_2 &= \int_a^b \left(\frac{1}{2} \varepsilon^2 - \varepsilon'^2 \right) dx + [\varepsilon \varepsilon']_a^b \\ \delta &= \int_a^b \frac{1}{2} \varepsilon''^2 dx.\end{aligned}$$

The model ψ_1 is positive, but the model ψ_2 is not—consider rapidly oscillating functions whose support is strictly contained in the interval (a, b) . Yet, ψ_2 is an excellent approximation (to order

η^4 in our notation) of ψ_1 . A non-positive energy can be a very good approximation to a positive one.

When the homogenization procedure delivers a non-positive model of the form ψ_2 , the above argument can be reversed to yield an equally accurate approximation ψ_1 that is positive. This is what we meant by ‘regularization’ in the last paragraph in Section 4.1. This idea will be further explored in upcoming papers in preparation: it can be used to ‘rescue’ non-positive homogenized models.

We find the reviewer a little pessimistic: our view is that non-positive homogenized models are equally useful, informative, and predictive as positive ones. We do agree that they need to be handled with care.

Reviewer As it is, the proposed effective model (33) is not correct and cannot be used for computing the equilibrium configuration. This is a serious concern and a stern warning is necessary for not helping the propagation in the scientific community of dubious asymptotic models.

Authors It is true that the energy (34) cannot be used *as is* in numerical simulations, and we already included a prominent warning about this point, see the last paragraph in Section 4.1. It can still be used in numerical simulations after suitable regularization, see our previous answer, or in analytical work. We are preparing a series of papers on this theme.

Reviewer The chosen example appears thus not suitable for illustrating the method (at least up to the second order) and I suggest to use an alternative one where the computed effective model remains positive.

Authors We disagree with this conclusion, see above. In any case, the new ‘Timoshenko’ example delivers a positive-definite energy functional W_{Tm} .

Reviewer Technical assumptions (see (24) or (61)) over the mean value of the corrector are needed when applying the method. The chosen assumptions are reasonable but nevertheless arbitrary: capturing upper nodal displacement instead of the average nodal displacement could also be a reasonable choice for someone desiring to apply forces on the beam from above. Some weight factor could also be attached to the nodes in (24). It is not clear to me whether the result (33) would have been the same (at second order) when using these alternative assumptions. I suggest the authors to check that point.

Authors We fully agree with the reviewer comment on the arbitrariness of the assumptions (25) and (62): in the presence of external loads applied at the interior nodes, the weights in the averaging rule (25) need to reflect the distribution of these external loads. When there are no external loads applied at the interior nodes, different choices for the weight factors in the average (25) will lead to different energy functionals that are equivalent to one another, as these models ultimately describe the same microscopic solution.

More specifically, to answer the reviewer’s question: the resulting energy (34) will have a different algebraic expression for different averaging rules, because the resulting macroscopic strains will be associated with different choices of the neutral axis, and will therefore differ from one another (except at dominant order). We can nonetheless anticipate that the alternative forms for the energy (34) can be mapped to one another by working out the correspondence of the strain measures.

We have added a remark on the arbitrariness of this choice in the paragraph below Eq. (25) but prefer not start a discussion of this side topic in the paper (this question is not specific to our homogenization method and could have equally been discussed in any previous paper on the homogenization of elastic trusses).

Reviewer In conclusion I suggest to publish the paper after discussion of the different points mentioned above and the modification of the illustrative example.

Reviewer 2 (Damiano PASINI)

The paper presents an asymptotically exact, second-order homogenization scheme for the linear analysis of periodic structural systems, such as truss-like materials, namely lattices. The paper

address an existing gap in the current literature. While asymptotic homogenization is well established and a wealth of works exist for periodic composites, some aspects are still poorly addressed and to certain extent overlooked. These span the inclusion of boundary terms and pre-stress (and pre-strain) to the modelling of spatial variations (yet slow modulations) of elastic and geometric properties in higher-order contributions. The paper builds upon a previous work of the authors on higher-order non-linear asymptotic expansion, which is here applied and tailored to the analysis of linear elastic structures with the potential of further extension to their non-linear periodic counterparts.

The work stands on a solid mathematical foundation which is abstract and generic in formality. It covers both periodic continua and discrete systems, and it holds generality of application to structures with periodic elements of higher dimensions, from 1D beam-types, 2D plate-types, to 3D spatial trusses. The key aspect of the work is the theoretical formulation which does not replicate that of classical methods, which typically start from the equations of equilibrium and express the displacement in the standard form of a series expansion, rather it is directly and interestingly conceived at the energy level.

Reviewer While I don't have specific comments to bring forward on the technical formulation, which I find robust and well explained, I have a constructive suggestion on the definition of some assumptions. In particular the concept of slow variation of elastic and geometric properties. It would be appropriate to articulate on what can be considered “slow” as opposed to “fast”. Some quantitative simple analysis to address this aspect might be useful here. For example, can the authors quantify what is the % of deviation from the ideal asymptotic solution that would occur for a prescribed set of modulations/gradients (from slow to fast) of properties?

Authors In the absence of convergence estimates, the only way to answer this question is to carry out a numerical convergence analysis (i.e., to generate numerical solutions with finite gradients and compare to the predictions of homogenization). This is a very significant work, which we will be presenting in a follow-up paper, currently in preparation.

Reviewer The paper is also well written despite some minor typos dispersed in the text such as “the the”, “any dependence take places”, and some others.

Authors We have fixed these two plus a couple others, thank you.

Reviewer 3 (Anonymous)

The authors of this paper propose a higher-order homogenization scheme for discrete structures in the framework of linear elasticity. The study relies on a two-scale expansion (slowly and rapidly varying quantities) asymptotic homogenization approach.

The main strengths of this approach are: (i) the method is applicable to any given discrete microstructure (also extendable to periodic continua); (ii) it is energy based, which means that, with a set of equilibrium equations, they also automatically retrieve boundary conditions; (iii) the model allows for pre-stress and slowly spatial variation of the elastic and geometrical properties of the microstructure.

This is an adaptation of an earlier work of theirs in the framework of nonlinear elasticity and the algorithm for the linear elastic case is also distributed as an open-source library named shoal.

Calculations are carried out systematically and clearly. The research is fair and interesting so that acceptance for publication in Journal of Theoretical, Computational and Applied Mechanics is recommended with the following remarks.

Reviewer In the “truss lattice” example analysed in Section 4.1, it is assumed to have an equivalent infinitely extended 1D beam model. What would have happened if the authors had assumed a 2D equivalent model? Would this assumption have required considering an infinitely extended lattice in the e_2 direction as well?

Authors The homogenization method works for arbitrary dimension. Starting from a lattice that has infinitely many cells in both the e_1 and e_2 directions, it is indeed possible to derive an equivalent 2D elastic continuum. We reserved these more advanced examples to a follow-up paper.

Reviewer Would the resulting 2D model be a general equivalent continuum that automatically particularised to the 1D beam model under the usual slenderness assumptions?

- Authors** In principle, an infinitely long strip comprising n cells in the transverse direction can be equally homogenized as a 2D slab or as 1D rod, and the two models should agree in the limit $n \gg 1$. However, the case $n = 1$ treated as an illustration in our paper cannot be approached by a 2D continuum since the boundary effects on the upper and lower sides would be dominant: 1D homogenization is then the only way to go.
- Reviewer** Since some structures would be well approximated by considering only the leading order terms, while others may require a higher order than the second to produce good results; does the approach suggest (or have the authors considered) a method to estimate the optimal order for truncating the expansion once a structure is given?
- Authors** This is an interesting remark. For simple problems, the successive approximations will deliver a more and more accurate picture, and it is up to the user to stop based on an accuracy target. For more difficult problems, however, when the leading order model is degenerate for instance, including the gradient correction is necessary. This can only be decided based on the inspection of the properties of the successive models, on a per-case basis.
- Reviewer** Does this model allow for the possibility of being extended to produce micromorphic models like the Mindlin-Eringen micromorphic model, the Cosserat model, or the microstrain model?
- Authors** Yes, it is possible to arrive at different types of models by choosing a different initial starting point (assignment of the \mathbf{y} versus \mathbf{l} degrees of freedom). The paper is already quite long, and we prefer not to include additional illustrations, but the general idea is illustrated by the new section on the Timoshenko model (§4.3).
- Reviewer** The reviewer also suggest to add the following reference: Bacigalupo, Andrea. "Second-order homogenization of periodic materials based on asymptotic approximation of the strain energy: formulation and validity limits." *Meccanica* 49.6 (2014): 1407-1425.
- Authors** We have added this reference in the introduction, thank you for the suggestion.
- Reviewer 4 (Jean-François GANGHOFFER)**
The paper deals with asymptotic higher-order homogenization of architected materials modeled as structural beam elements at the microscopic level. The framework of linear elasticity is adopted at both micro and macro levels. The paper is clearly interesting for the reader of the journal; there are a number of issues the authors should address while revising their paper.
- Reviewer** Especially, it remains unclear to what type of theoretical / numerical results the proposed methodology may lead, considering especially finite-size effects.
- Authors** It is correct that finite-size effects are used as a motivation to derive higher-order gradient models, but we do not provide specific application examples where these higher-order models are used to address finite-size effects. Doing so requires solving these models numerically and addressing layers forming at the boundary: this is still a very substantial work that we cannot address in this first paper. We hope that this will be covered extensively in a series of upcoming papers which use the present paper as a starting point.
- Reviewer** Major issues
Is W introduced in (4) size-dependent or intrinsic to a supposedly existing lattice unit cell?
- Authors** In preamble, we disagree with the use of the word 'major' to characterize this list of issues. Eqs (4-5) is a generic form of the energy, see (32-33) for a specific expression. The strain E entering in W is a function of η (we expand in series of η): the size-dependence is present in the model we start from, and it propagates to the homogenized model. We added a reference to (32-33) below Eqs (4-5) to clarify this point.
- Reviewer** The paper is not organized into a logical manner, since the main results of the homogenization method are announced in section 3, but one has to wait Section 5 for their proof.
- Authors** The organization of the paper is not linear but it is unfair to call it un-logical. Its organization is clearly announced by the section headings and the multiple references to equations. The proposed organization has the advantage of making the main results accessible while keeping the

calculations details available to the interested readers. An earlier version of the manuscript was organized in a linear manner, and the current organization appears to be much more preferable.

- Reviewer** How is periodicity of the lattice in Section 4 accounted for in the continualization method?
- Authors** This comes from Eq. (23), which is a sum over the repeated bar pattern. It is the periodicity that allows this discrete sum to be rewritten in (33) as a (continuous) integral—in this integral, the remaining sum over i refers to the 5 types of bars in Figure 2. We added a statement just before Remark 7 to point this out more clearly.
- Reviewer** The continualization rule below Eq. (32) seems unusual, since one normally convert powers of the small parameter (2 in 2D, 3 in 3D) into the continualized Riemann integral.
- Authors** We believe the reviewer refers to the fact that the volume of the unit cell, η^d in our notations, enters as a scaling factor in front of the Riemann integral. This is also the case in our example, see the coefficient η^1 in the denominator of (33) (this example is in dimension $d = 1$).
- Reviewer** It is not clear whether the obtained continualized energy reflects or not size effects. If so, one may speak of apparent properties (tending to homogenized ones only for infinite lattices). It is not clear how finite size effects are quantified in the model. Such effects may be reflected by the importance of boundary effects on the apparent mechanical properties; they may also lead to a non-standard macroscopic behavior with the appearance of higher order terms. All these aspects need better explanations.
- Authors** The whole point of our paper is to address the higher-order terms capturing the gradient effect. As for the prediction of apparent mechanical properties, this requires *solving* our homogenized models in specific geometries which, as mentioned above, is beyond the scope of this paper. Take the example of a lattice that is infinite in one direction and, say, $n = 20$ cells wide along the other direction: we could derive an equivalent 2D elastic medium for this lattice, and solve it along the width to capture how its equivalent bending properties depend on n (finite-width effect).
- Reviewer** The authors can refer to following relevant recent papers on the topic:
- Analysis of surface effects based on first and second strain gradient mechanics. Mawassy et al., 2022. *Mechanics of Materials* 175(13):104462.
 - Continualization method of lattice materials and analysis of size effects revisited based on Cosserat models. Alavi et al., 2022. *International Journal of Solids and Structures* 254-255(3):111894.
- Authors** We thank the reviewer for the suggestion. We prefer not to add these two references to our paper: they discuss interesting size effects but are not specifically using an asymptotic homogenization method, which is our focus here. The literature on size effects in general is vast.
- Reviewer** Is there any internal length associated to the strain gradient model developed in section 5.2?
- Authors** Indeed, the mesh size enters into the coefficients associated with the gradient, by dimensional reasons. This can be seen from the presence of the coefficient η^2 in (36).
- Reviewer** In what situation is such a strain gradient model needed? Is it e.g. adequate to describe a micrograding of the unit cell? Could the authors provide a relevant (even simple) example to illustrate such a situation?
- Authors** This has been discussed in our response to another reviewer above: the strain gradient terms are useful in broad circumstances to improve the accuracy of the solution when the separation of scale is imperfect (as highlighted by numerous papers cited in the introduction, starting with Boutin 1995). Alternatively, they can be required in specific circumstances/under special scaling assumptions, when the leading-order is degenerate (see for instance the work of Seppecher on pantographic materials). The main focus of the paper is on the homogenization method itself and we would prefer not to add more specific application examples. We have added a new illustration per request of the other reviewers (new Subsection 4.3: Timoshenko beam) and the paper is quite long already.
- Reviewer** The present referee is wondering of the connection of the developments presented in Section 7

with the core of the paper; are those standard results for the homogenization of continua or do they present some novelty in line with the continualization method exposed in the previous sections.

Authors This section shows that our method is consistent with known results in the special case of a *homogeneous and continuous* medium: there is no claim for novelty in this section, the goal being to check consistency with existing results. We believe this is clear from the section heading, from the introduction ("gives similar results to the classical approach"), from the way earlier work is cited in this section, and from the discussion in Section 8. We are afraid we do not see what we could change.

Reviewer Minor issues

It seems that a single space variable X is employed, whereas double scale asymptotics clearly requires two spatial scales. It is thus not clear in the entire paper whether (and how) the authors perform a double scale asymptotic expansion.

Authors The fast and slow variables are present in the homogenization of a continuous medium, see Section 7 and Eq. (52) in particular. Most of our paper is concerned with the discrete setting, in which the fast variable is replaced by a *discrete* index, such as the oscillating sign \pm in Eq. (24): the nodes in the discrete beam are identified by a continuous (slow) variable X and by a discrete (fast) index \pm .

Reviewer It looks from the example treated in p. 8 that the vectors \mathbf{m} represents rather geometrical parameters (instead of material ones).

Authors In Eq. (33), \mathbf{m} appears to be the argument of the variable stiffness k : it captures elastic inhomogeneity and not geometric ones.

Reviewer It is contrary to standard notation to denote E (upper case letter) the microscopic strain.

Authors We are not sure what alternative notation the reviewer has in mind, but we decided that ε would be unfortunate for spring elongation.

Reviewer Below Eq. (2), the meaning of the subscript notation E_l, E'_l should be explained. Why are the introduced quantities not also to depend on l ?

Authors The l in subscript is non-bold, and is a label that is different from the variable l appearing in the left-hand. We agree that this could be confusing and are now referring to Table 4 to make this clear.

Reviewer The notation of the 'delta's' with double indices should be better explained.

Authors The notation was explained in the legend of Table 4, now moved in the paragraph immediately before Table 4. We have also added a specific examples that should help clarify it further.

Reviewer The paragraph below Eq. (18) is unclear to the reader.

Authors This paragraph has been rephrased, we hope it is clear now.

Reviewer In Section 4.1, the notation for the lattice nodes are not explained (arguments of vector X_a below figure 2).

Authors In the paragraph with heading "Discrete model", we changed the (X_1, X_2) notation defining $X_{\alpha\pm}$ to an $X_1\mathbf{e}_1 + X_2\mathbf{e}_2$ notation, hoping that this was the source of the confusion.

Review of version 3

Permalink: hal-04112136v3

Reviewer 1 (Pierre SEPPECHER)

Reviewer Let me start with my conclusion: The proposed paper is useful because it gives a good tool for skipping many tedious computations, hence it should be published. However I remain doubtful about the homogenization framework it promotes. I comment below some of the authors answers:

- “Comparing the respective merits of different models is beyond the scope of our manuscript, which is focused on carrying homogenization for a specific assignment of macroscopic vs. microscopic strain.” I think that homogenization is precisely determining the merit of different macroscopic models. Choosing a type of model is not fundamentally different from fixing its parameters: for instance, assuming that the considered beam is of Euler-Bernoulli and not Timoshenko type is equivalent to assuming a null value for some of the coefficients of a more general model.
- “We do hide the detailed microscopic solution (y) in the homogenized model, while accounting for it accurately. We do not see any contradiction between ‘hiding’ (we eliminate the quantity y , by solving an elastic problem) and ‘taking it into account’ in fact, doing so is precisely the point of homogenization. Dimension reduction does the same, by hiding the details of deformation in the cross-sections, while resolving them accurately under the hood and delivering an effective energy that accounts for them.” It is not a question of “accounting for them”. Of course we need to do that. It is the question of providing a macroscopic model which contains an intrinsic length of order of y and so aimed to give details of the equilibrium state at the scale of one cell or less. Moreover, even if one assumes that there exists some deus ex machina which regularizes the solution without sensibly modifying its energy (?!?), the provided “better” approximation of the energy can be used only if one controls all other terms of the total energy at this order: for instance, the position of the macroscopic boundary or the position of the support of applied external forces must be known with a precision much better than the cell size...
- “Note: we are assuming that the reviewers means inconsistency rather than inconstancy.” The authors are right. Maybe I was thinking of the constancy of this inconsistency in the literature!
- “A non-positive energy can be a very good approximation to a positive one.” The authors give an example to support this assertion which clearly shows the need of some precision: indeed, as they say themselves, this is not true for rapidly oscillating functions.
- “We find the reviewer’s a little pessimistic: our view is that non-positive homogenized models are equally useful, informative, and predictive as positive ones. We do agree that they need to be handled with care... It is true that the energy (34) cannot be used as is in numerical simulations.” Pessimistic or realistic? The problem is not only a numerical one but also a physical one. There must be a physical reason (and not only a “suitable regularization”) which prevents the rapid oscillations that are predicted by the non positive energy. This extra energy term will become as important as the improvement obtained by the higher order homogenization scheme.

Reviewer 2 (Damiano PASINI)

The authors addressed my previous comments and I have no further recommendations.

Reviewer 3 (Anonymous)

The authors’ responses have addressed the reviewer’s concerns satisfactorily, leaving no additional comments to be made. Hence, I recommend accepting this submission for publication in the Journal of Theoretical, Computational and Applied Mechanics.

Reviewer 4 (Jean-François GANGHOFFER)

The authors have answered the issues I raised in my report in a satisfactory manner; the paper can accordingly be published.

Editor’s assessment (Laurence BRASSART)

The paper proposes a generic higher-order homogenisation method based on two-scale expansion to calculate the effective properties of linear discrete elastic structures (lattices). The method is based on energy minimisation with respect to the microscopic degrees of freedom and can account for boundary conditions as well as pre-stresses, which have often been overlooked in previous works. In addition, the authors provided a general numerical implementation of the procedure based on the symbolic calculation language Wolfram Mathematica. All reviewers found the paper of interest for the readers of the journal. Reviewers raised a number of minor and major points that needed to be addressed in a revised version. After revision, all reviewers recommended the paper to be accepted for publication. Further comments of Reviewer 1 on the authors’ response have been noted.

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