DOI: 10.13009/EUCASS2019-780

Multiscale structural simulation of metamaterials under large strains. Generation of the RVE behaviour

Francisco Javier San Millán Fiel, Francisco J. Montáns***
** Instituto Nacional de Técnica Aeroespacial (INTA)*
Ctra. Ajalvir Km 4, 28850 Torrejón de Ardoz (Spain), e-mail: sanmillan@inta.es
*** Escuela Técnica Superior de Ingeniería Aeronáutica y del Espacio (ETSIAE)*
Pza. Cardenal Cisneros 3, 28040 Madrid (Spain), e-mail: Fco.Montans@upm.es

Abstract

Metamaterials are designed to achieve the desired properties (structural, optical, acoustic absorption, etc) not found in ordinary materials, and possess in general an internal micro-structure whose design drives the aimed properties of the metamaterial at the macro level. Structural simulation of metamaterials is complex because it must consider at least two scales addressing both the analyses of the internal structure and the macroscopic structure, so it is often solved by using Multi-scale Finite Element Analysis (FEA). When the structure undergoes large strains multiscale FEA is usually prohibitive in computational cost, so in this paper an efficient procedure is proposed that offers considerable time savings, while keeping at the same time a good accuracy.

Keywords: Metamaterials, Auxetics, negative Poisson´s ratio, Multiscale Finite Element Analysis

1. Introduction

A metamaterial is an artificial material designed to achieve a set of desired properties at continuum level: structural properties, optical properties, acoustic absorption, etc [1][2]. Metamaterials expand boundaries of conventional materials and are at the moment a very active research topic because of its potential economic benefit in the near-term future, and because they represent a clear innovation driver with many diverse applications [1]. Metamaterials possess in general an internal micro-structure of certain complexity that is repeated in space, the design of this internal micro-structure drives the properties of the metamaterial at macroscopic level.

A simple classical example of metamaterial (in this case for a structural application) is a honeycomb sandwich panel, often used in aero-space applications to achieve high stiffness and strength, while minimizing the weight of the panel. Another structural example is the so called auxetic metamaterial [3][4][5][6] that have an unconventional mechanical behaviour, namely a negative Poisson´s ratio, so when subjected to tensile loads, it presents dilatations in the transverse directions. This unconventional behaviour is interesting for many applications such as impact energy absorption [4][7][8], improved fatigue and fracture mechanics properties [4], active structures [9], etc.

The structural simulation of meta-materials is of certain difficulty because it has to consider both the analysis of the internal structure (the micro-structure responsible of the desired properties), and the analysis of the macro-structure itself: a box, a reinforced structure, etc [10][11]. A technique quite often used is the multi-scale Finite Element Analysis (FEA) [1], traditionally used, for example, in the analysis of dislocation progression in metals.

When the structure undergoes large strains multiscale FEA of the metamaterial is prohibitive in computational cost terms, and it often presents convergence problems when using implicit FE solvers. We herein propose an efficient procedure for the multiscale metamaterial FEA through a continuum mechanics bridge. The idea is to get the structural properties of the structure at micro level from Virtual Tests of a representative volume element, deriving the non-linear behaviour of the micro-structure under possible combinations of different deformation modes, including all types of

DOI: 10.13009/EUCASS2019-780

nonlinearities, namely geometrical, material and contact between cell walls. These curves are then used by the WYPiWYG (**W**hat **Y**ou **P**rescribe **is** **W**hat **Y**ou **G**et) technique developed by our group to derive the constitutive non-linear equations for each stress integration point at the continuum level [12][13].

The advantage of the procedure is the considerable time savings achieved since the macro FEM is extremely efficient from the numerical point of view, while keeping at the same time a high accuracy.

2. Proposed approach for efficient simulation of metamaterials at large strains

When the metamaterial undergoes large strains, a multi-scale FEA becomes computationally difficult and costly, since iterations are needed for each integration point and load step, both form macro FEM to micro FEM and reverse. At large deformations in the structure, the metamaterial cell walls undergo large deformations (probably inelastic) and contacts between them may increase the difficulty in obtaining a solution. This creates further difficulties in overall model convergence and limits the application of multi-scale FEA for full-scale structures.

The paper proposed an efficient procedure for multiscale metamaterials FEA at large strains. The idea is to obtain the structural behaviour for deformation modes at the micro level from virtual (numerical) tests of a representative volume element (RVE), deriving the non-linear behaviour of the micro-structure under possible combinations of the different deformation modes, upon the idea that the behaviour of the metamaterial in a structure is mainly dominated by the primal deformation modes present in a linear analysis. Therefore, couplings between modes at very large strains are neglected. The considered deformation modes are expansion and/or compression axial deformations along the three axes, and shear deformations in the three planes. This small RVE of the metamaterial is modelled by the FE technique and analysed using the implicit solver MARC [14], to get the non-linear mechanical behaviour of the RVE (load-deformation curves, etc.). To ensure RVE applicability and proper modelling, different FE of intermediate scale (sets of RVEs) are created and analysed with MARC. The behaviour of these intermediate FEMs are compared to the behaviour of the RVE, to validate the RVE FEM through mesh convergence procedures. Pre/post has been made using PATRAN [15].

Once the RVE FE has been validated, the results are then input to the WYPiWYG model procedure [12][13], to derive the constitutive non-linear equations at continuum level, at macro scale. The macro FEM will be solved by using the in-house solver DULCINEA.

The advantage of the procedure is the considerable time savings achieved since this macro FEM is extremely efficient from the numerical point of view, while keeping at the same time a high accuracy, and an adequate modelling of non-linear effects that results in an accurate representation of the behaviour of the macro-structure, enabling its application for big structures. The classical macro-micro and micro-macro iterations, required in large strain multiscale FEA are no longer required using the procedure proposed in this paper.

3. Benchmark studied: an auxetic sandwich

Auxetics are unconventional materials that show negative Poisson's ratio, so they get fatter when stretched (they show transversal expansion when stretched along longitudinal direction), or narrower when compressed [3][4][5][6]. The unconventional structural behaviour of auxetics yield, as a result, improved mechanical properties (most of them highly dependent on material Poisson's ratio): excellent behaviour regarding impacts, high indentation resistance, superior energy absorption capacity, improved fatigue behaviour, increase of material fracture toughness, acoustic absorption improvements, active structures (synclastic curvature when the structure is submitted to in plane bending).

The first benchmark selected for our study is an auxetic sandwich panel designed for improving blast resistance of armoured vehicles [7]. In Figure 1, the design of such a sandwich is shown. The initial RVE, or the unit cell that it is repeated many times, is shown in Figure 2, being its main dimensions: l_X (total length along X axis) = 50.35 mm, l_Y = 20 mm, thickness t = 0.6 mm, and $l_{X\,edge}$ (upper and lower edges length along X axis) = 34.35 mm. The angle between the upper and lower edges and the oblique ones is 50º.

DOI: 10.13009/EUCASS2019-780

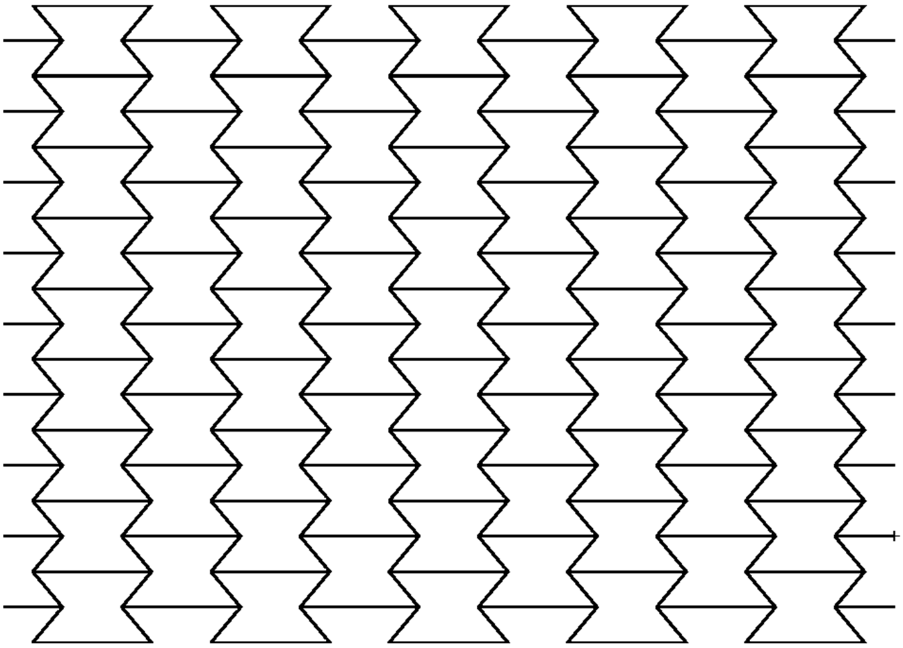

Figure 1: Auxetic sandwich design

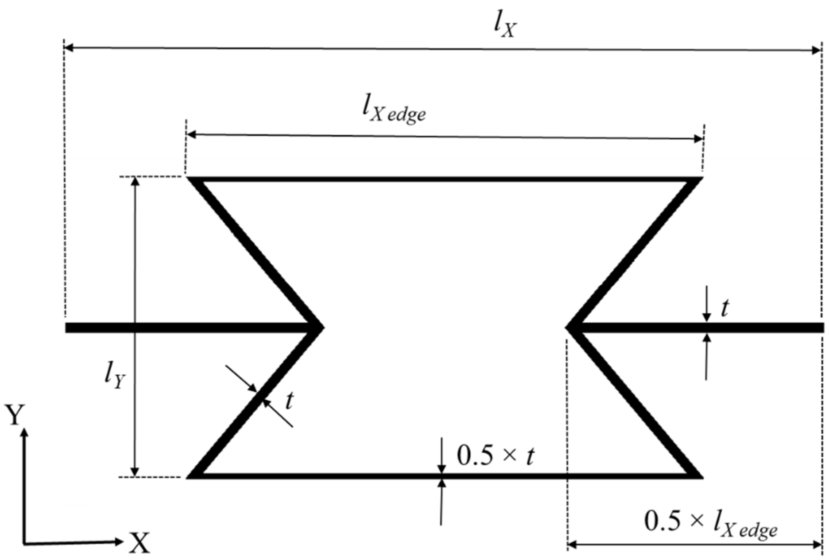

Figure 2: RVE (unit cell) of the auxetic sandwich

4 Numerical models

The behaviour of this auxetic sandwich is mainly bi-dimensional [7]. The 3D effects (transverse direction strain and shear) are simpler because they correspond to those of an ordinary material. Thus, for simplicity, in this paper only 2D FEA results are presented. The elements used for the 2D finite element analyses are of thick shell type (element 75 in MARC terminology), and the material model is hyperelastic following a neo-Hookean formulation:

$$W = C_{10}(I_1 - 3) \quad (1)$$

$$I_1 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 \quad (2)$$

DOI: 10.13009/EUCASS2019-780

$$\lambda_i = \frac{L_i + \Delta L_i}{L_i} = 1 + \varepsilon_i \tag{3}$$

Being W the strain energy potential, I_1 the first strain invariant, λ_i the stretch ratio along i direction, and ε_i the engineering strain along i direction. The neo-Hookean model is based on statistical mechanics and thermodynamics and it is adequate for modelling plastics, rubber-like substances, etc.

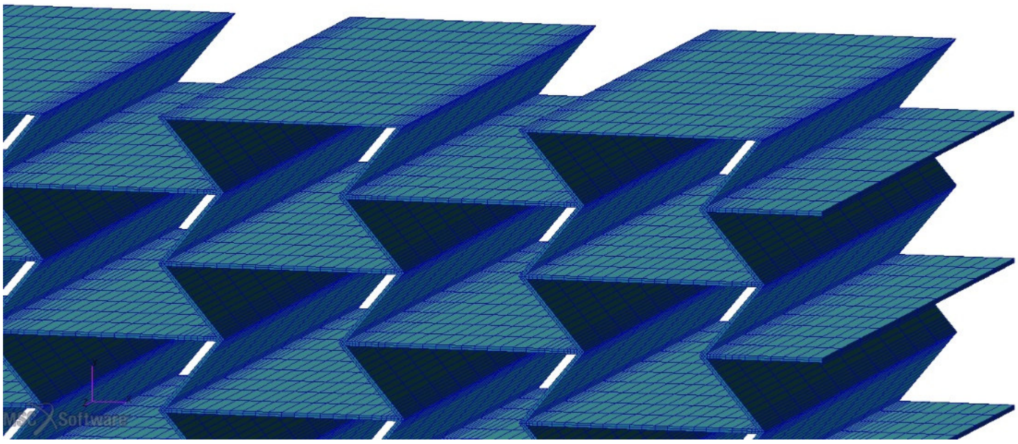

Figure 3: Detail of solid FEM of the sandwich panel

The material parameter values used in the MARC FEM are $C_{10} = 1.13 \times 10^8$ Pa and Bulk modulus = 1.4×10^{11} Pa, so the material behaviour is nearly incompressible. Solution used is non-linear static accounting for large displacements and large strain effects. In Figure 4 we show the mesh used for the unit cell.

4.1 Deformation modes studied

In this study and because the problem is 2D the most relevant deformation modes are in plane: axial strain along X axis, axial strain along Y axis, and in-plane Shear XY.

Loads are applied to the FEM as imposed displacements. For compatibility reasons boundary conditions have to be used for the FEM ensuring that unit cell nodal displacements are compatible with the nodal displacements of the surrounding unit cells, so the unit cell is a RVE. So for this reason in the axial problems (both along X and Y axes) MPCs (Multi-Point Constraints) linking U_Y displacement have been used in the upper and lower edges of the RVE (see Figure 4).

DOI: 10.13009/EUCASS2019-780

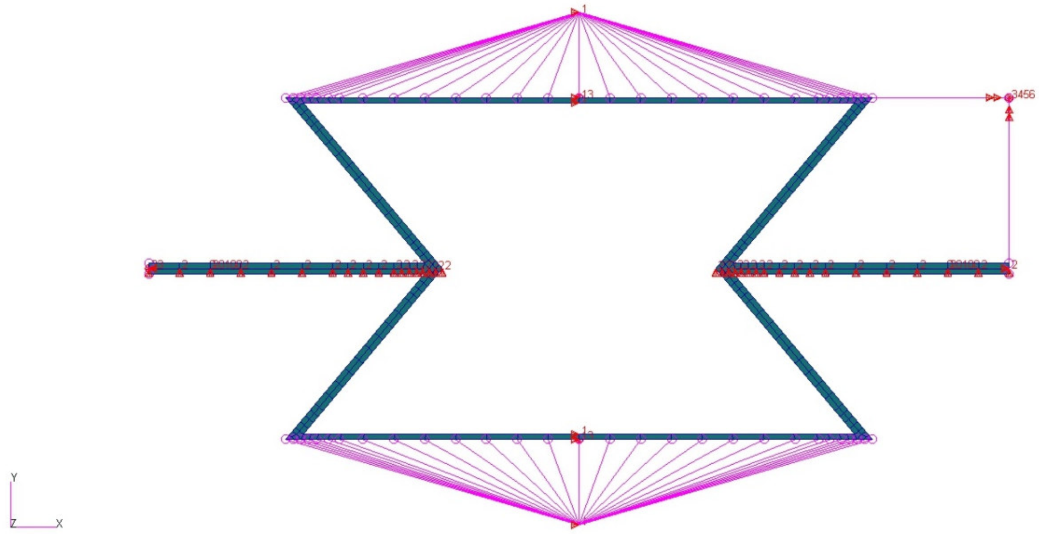

Figure 4: Unit cell with axial loads (U_X displacement), symmetry boundary conditions, and showing the auxiliary node

In Figure 4, axial loads correspondent to 20 mm stretching along X axis (U_X = 10 mm at right end nodes and U_X = -10 mm at left end nodes), and symmetry boundary conditions, are also shown. It is clear that for axial cases only a quarter of the RVE FEM would be enough for the analysis, but for practical reasons (the FEM is used for the Shear XY mode analysis as well) the complete RVE FEM has been used. An auxiliary and non-structural node, linked via MPCs to the RVE FEM, has been used for the derivation of XY and YX Poisson`s ratios (ν_{XY} and ν_{YX} respectively).

In plane XY shear is far more difficult to simulate mainly referring to compatibility conditions (lack of symmetric displacements, slight coupling between shear loads and axial deformations, etc). For the moment simulations several approaches have been checked with acceptable correlation between the RVE FEM and the intermediate FEM (see next section).

5. Intermediate FEM results and RVE FEM validation

Several intermediate FEMs (2D and 3D) have been generated and analysed: 3 × 5, 5 × 7, and 7 × 9, being the first number the number of "columns" of the sandwich FEM, and the second number the number or "rows". In Figure 5 the 5 × 7 2D FEM can be seen. Boundary conditions (symmetry in left and lower sides), applied displacements U_X at the right side, and MPCS linking U_Y (only in the upper part of the FEM) are also shown in the Figure.

DOI: 10.13009/EUCASS2019-780

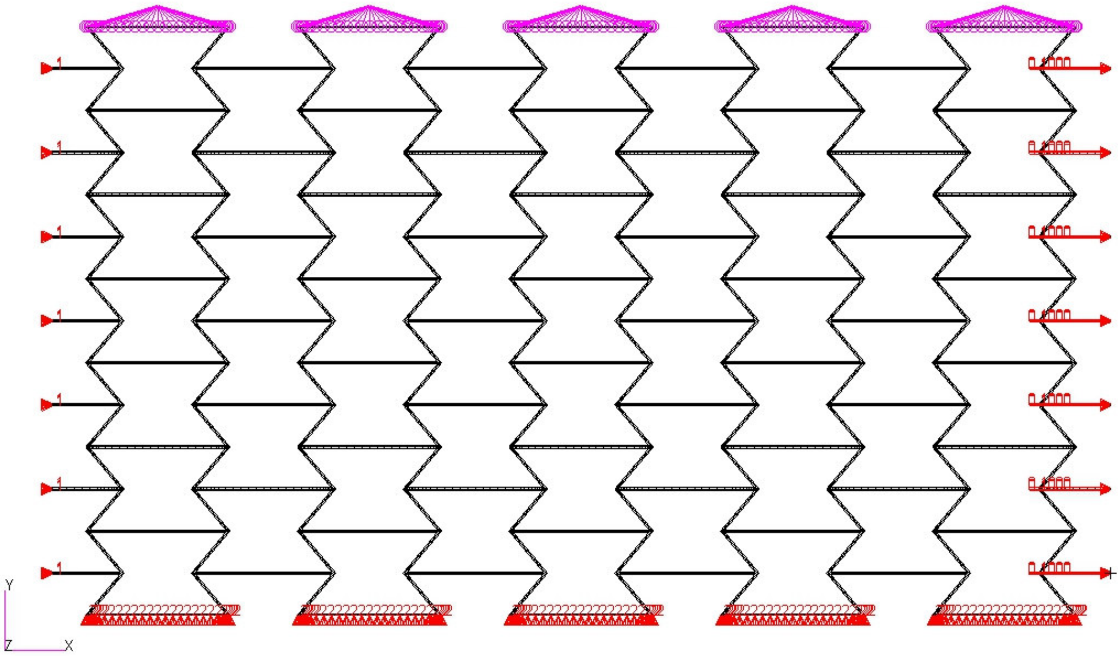

Figure 5: Intermediate (5 × 7) 2D FEM

Validation of the RVE FEM is performed in 3 steps:

- Correlating the reaction force – displacement curves (being the reaction force the forces internally applied by MARC to achieve the imposed displacements) in both FEMs: RVE and intermediate ones for equivalent loads. For instance comparing the curve of RVE FEM when it is subjected to a 20 mm stretching along X axis with the curve result of the intermediate FEM analysis applying a stretch of 100 mm (20 mm × 5) along the same X axis.
- Correlating deformed shapes of both FEMs, for equivalent load conditions.
- Correlating the Cauchy stresses at both FEMs, again for equivalent load conditions.

Concerning the Axial deformation modes (U_X and/or U_Y displacements), the correlation is almost perfect. For instance in U_X cases in Figure 6 to Figure 8, the quick plots (deformed FEM + results fringe) showing VM (Von-Mises) Cauchy stresses σ_{VM} and transverse U_Y displacements are shown.

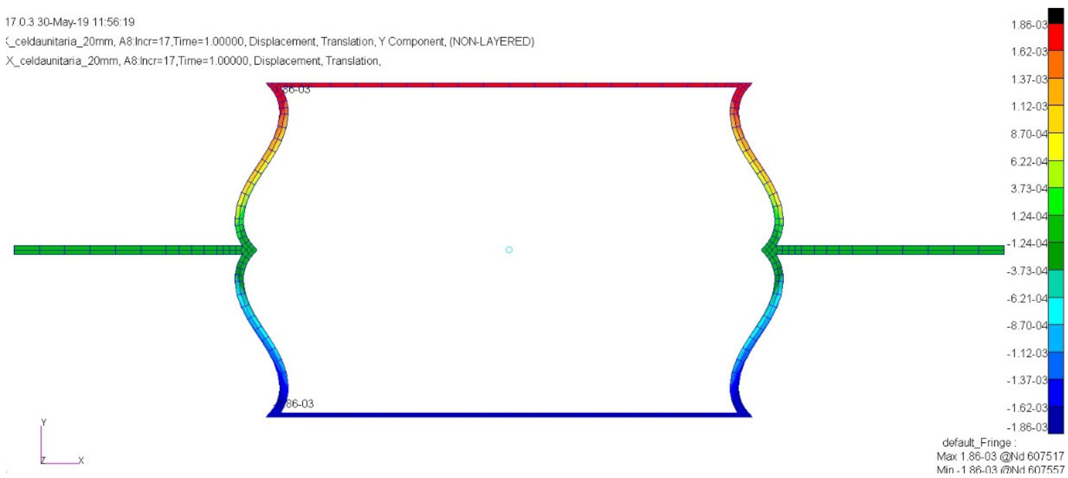

Figure 6: RVE FEM. Plot: deformed shape + σ_{VM} fringe

DOI: 10.13009/EUCASS2019-780

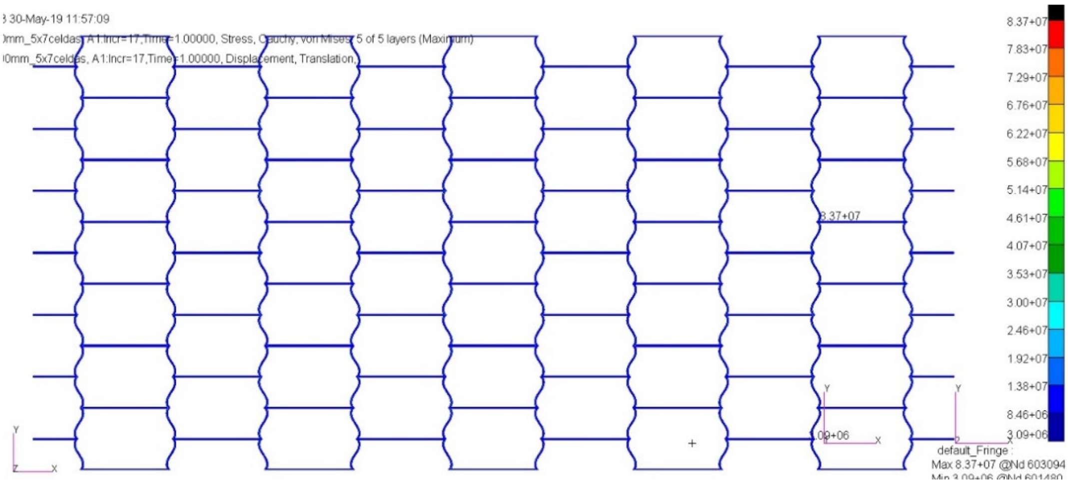

Figure 7: Intermediate FEMs (5 × 7). Plot: deformed shape + σ_{VM} fringe

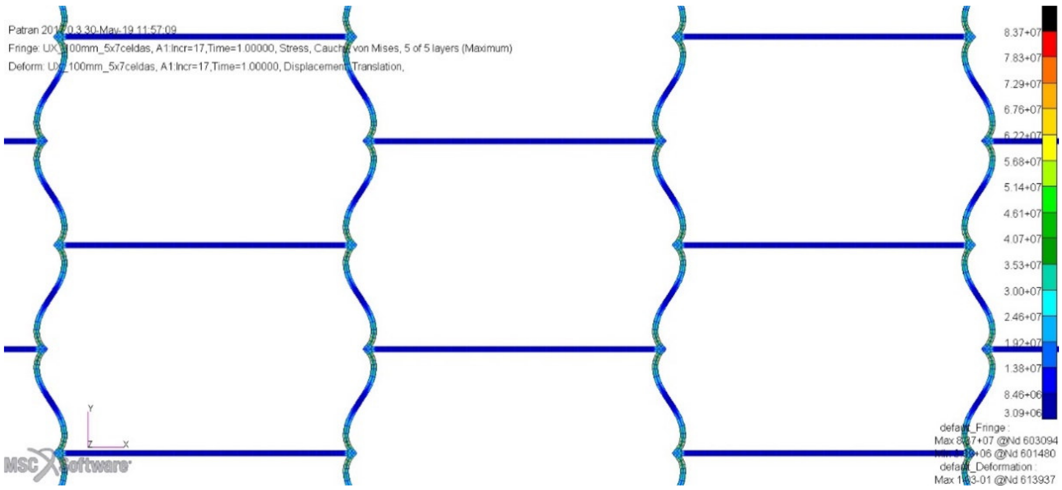

Figure 8: Intermediate FEMs (5 × 7). Plot detail: Deformed shape + σ_{VM} fringe

As it can be seen VM Cauchy stress σ_{VM} values are equal in both FEMs.

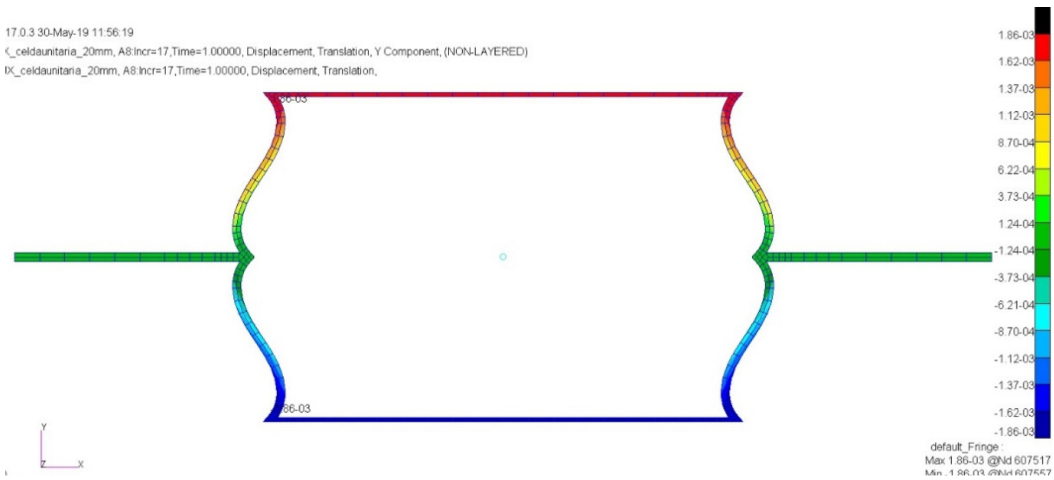

Figure 9: RVE FEM. Plot: deformed shape + U_Y fringe

DOI: 10.13009/EUCASS2019-780

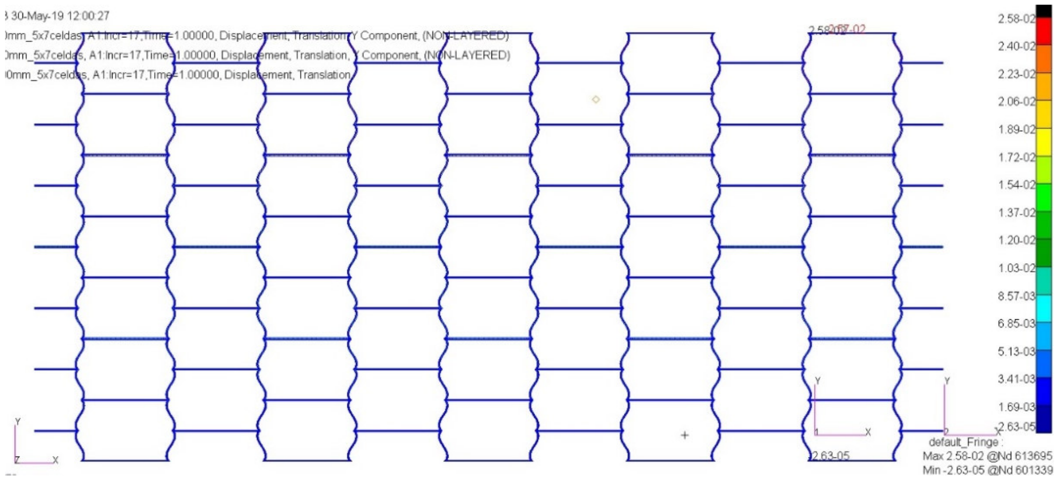

Figure 10: Intermediate FEMs (5 × 7). Plot: deformed shape + U_Y fringe

Concerning U_Y transversal displacement RVE FEM shows maximum U_Y of 1.8374 mm (at the upper edge) and minimum U_Y of - 1.8374 mm (at the lower edge), so the stretching of the RVE along transverse Y axis is 3.6748 mm. Intermediate FEM shows maximum U_Y of 25.724 mm (upper edge), lower edge is supported along Y axis (it is a symmetry plane in this case). The ratio between both U_Y values is:

$$\frac{U_{Y\ intermediate\ FEM}}{U_{Y\ RVE\ FEM}} = \frac{25.724}{3.6748} = 7 \tag{4}$$

7 is precisely the number or "rows" of the intermediate FEM, so the correlation concerning U_Y displacements between the 2 FEMs is excellent as well.

From the different load steps of RVE FEA for the load case of load along X axis (range from shortening of 15 mm to a stretching of 20 mm), the following non-linear constitutive curves are found:

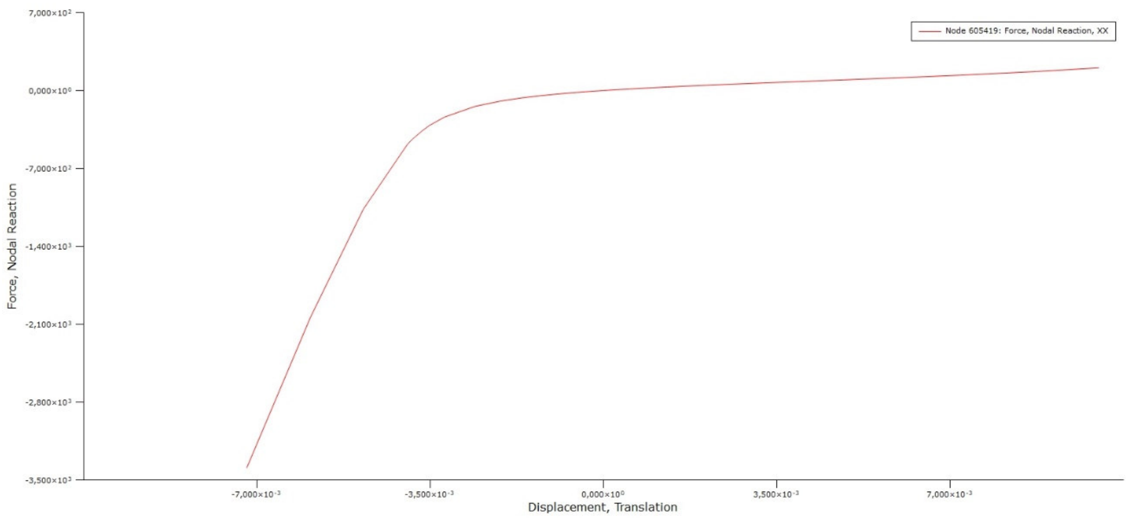

Figure 11: Relation $F_X - U_X$ (half the RVE stretching)

DOI: 10.13009/EUCASS2019-780

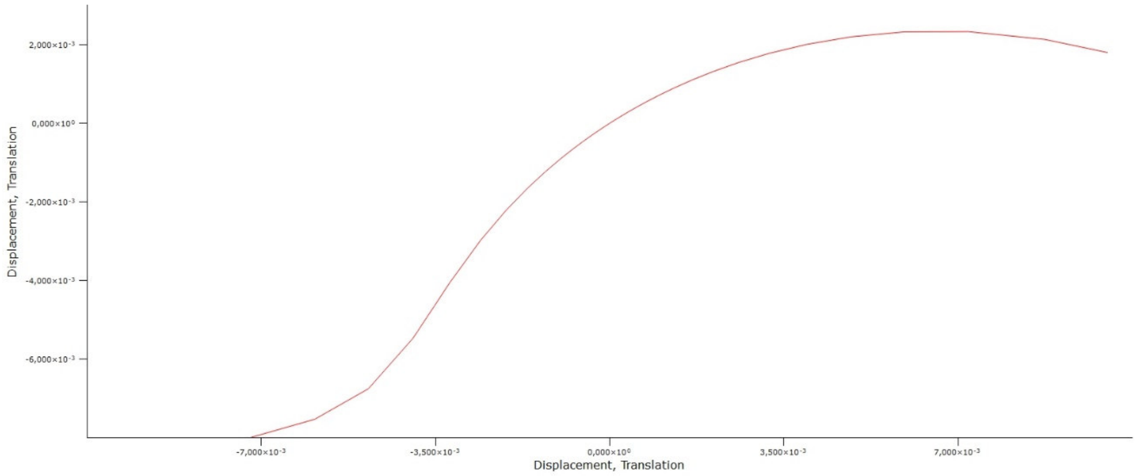

Figure 12: Relation $U_Y - U_X$ (equivalent to RVE non-linear Poisson´s ratio ν_{XY})

These curves, together with the curves result of the other load cases, are the constitutive equations needed as input to the WYPiWYG technique [12][13].

Similarly to the U_X load case, axial case of load along Y axis show excellent correlation between RVE and Intermediate FEMs. At the moment the correlation found for in-plane shear load case is acceptable but need further refinement work, especially when dealing with compatibility conditions used in the RVE FEM.

Once we have determined the behaviour of a RVE, including the boundary conditions needed to guarantee the scalability of the RVE (i.e. that 2x2, 3x3, etc linked unit cells give the same behavior per unit cell), we can use that representative behaviour to generate a continuum-based model that replicates it at every stress integration point during a finite element simulation. The continuum-based model is generated using the WYPiWYG technique, which was already fully tested in a wide range of nonlinear materials, isotropic [13][16][17], transversely isotropic [18] and orthotropic [19][20].

6. WYPiWYG technique and overall simulation scheme

The WYPiWYG technique [12][13], has been developed by our group to derive constitutive non-linear equations at continuum level, at macro scale, directly from experimental data, preserving the thermodynamics (i.e. preserving energy in purely elastic deformations). The macro FEM is solved by using the in-house solver DULCINEA or using a commercial finite element code as ADINA with the WYPiWYG material coded as a user subroutine.

The WYPiWYG procedure assumes a nonlinear stored energy decomposition motivated in the theory of linear composite materials. For the orthotropic case, for example we assume:

$$\Psi = \mathcal{U}(J) + \omega_{11}(E_{11}^d) + \omega_{22}(E_{22}^d) + \omega_{11}(E_{33}^d) + \omega_{12}(E_{12}^d) + \omega_{13}(E_{13}^d) + \omega_{23}(E_{23}^d) \quad (5)$$

where E_{ij}^d are the components of the deviatoric logarithmic strains in the material symmetries in the reference configuration (note that these are invariant quantities), J is the Jacobian determinant of the deformation gradient, and ω_{ij} are scalar-valued functions to be determined from experimental data following the WYPiWYG procedure. These functions are determined numerically as to reproduce the experimental data in the seven modes of deformation considered and which are parallel to those of the infinitesimal theory (for incompressible materials), but in this case capable of predicting any suitable nonlinear relation obtained from the virtual tests on the RVE. Material symmetries congruency [21] are not deemed necessary in this case.

The purpose of the work being performed currently is to demonstrate that, for a general macroscopic structure under generic loads, the reduced continuum-based model, is capable of accurately reproducing the behaviour of the structure at several orders of magnitude less that the cost of what is needed when using the structure considering both scales. These simulations are still ongoing research.

DOI: 10.13009/EUCASS2019-780

The overall simulation scheme of the methodology proposed in this paper is shown in Figure 11:

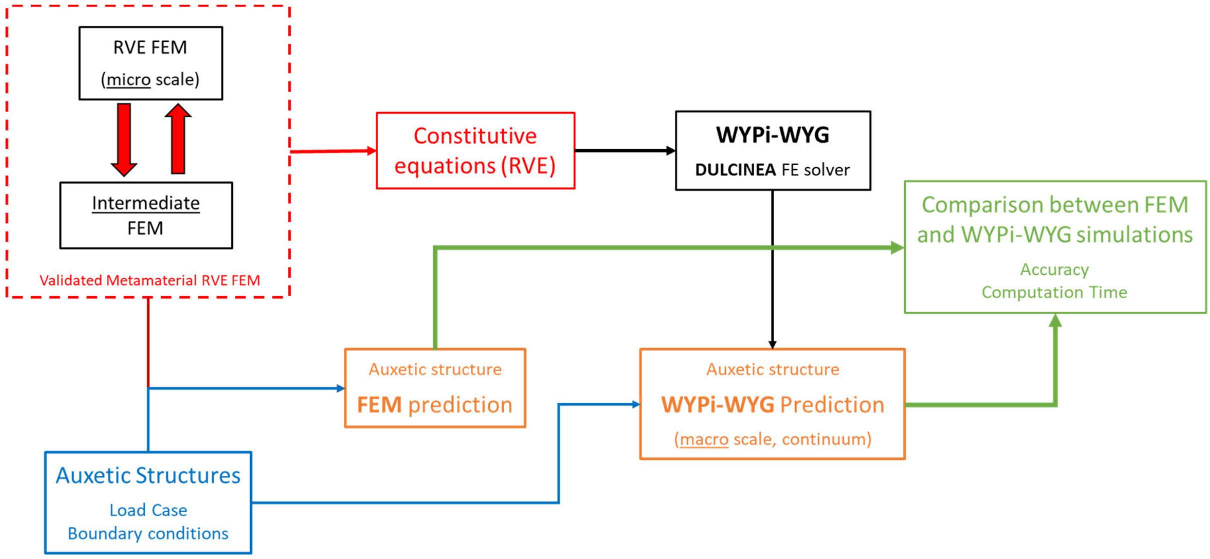

Figure 11: Overall simulation scheme

8. Conclusions and pending work

In this paper a methodology has been presented for large strains multiscale FEA of metamaterials. This kind of analyses, especially when dealing with large strains, are very costly in computational cost terms and present convergence problems. The proposed methodology combine non-linear FEA at different scales, with WYPiWYG technique developed at the ETSIAE University that derive the constitutive non-linear equations of the metamaterial at continuum level.

The benchmark used for this study is an auxetic sandwich. Different FEMs (2D and 3D) have been generated of the sandwich RVE (unit cell), and intermediate FEMs considering different sets of unit cells, and they have been solved with implicit non-linear solver MARC. Preliminary FEA results show an excellent correlation for the axial cases (load applied in the sandwich plane). At the moment the correlation found for in-plane shear load case is acceptable but need further work, especially when dealing with compatibility conditions used in the RVE FEM.

From the RVE validated FEMs all needed constitutive equations are derived and will be used in the near future as inputs of WYPiWYG technique and DULCINEA solver. To finally validate completely the proposed methodology, different structures will be modelled both by FEA and WYPiWYG/DULCINEA to show the accuracy, and efficiency (computation time) of the proposed methodology compared to conventional procedures.

Acronyms

- ETSIAE (Escuela Técnica Superior de Ingeniería Aeronáutica y del Espacio, Universidad Politécnica de Madrid, Spain)
- FE: Finite Element
- FEA: Finite Element Analysis
- FEM: Finite Element Model
- MPC: Multi-Point Constraint
- RVE: Representative Volume Element
- VM: Von-Mises

DOI: 10.13009/EUCASS2019-780

References

[1] Bishop-Moser, J., C. Spadaccini, and C. Andres, 2018. Metamaterials Manufacturing, Pathway to Industrial Competitiveness, MForesight (Alliance for Manufacturing Foresight) Report.

[2] González, C., J. J. Vilatela, J. M. Molina-Aldareguía, C. S. Lopes, and J. LLorca, 2017. Structural composites for multifunctional applications: Current challenges and Future trends, *Progress in Materials Science* Volume 89, 2017, pages 194-251.

[3] Ren, X., J. Shen, A. Ghaedizadeh, H. Tian, and Y. M. Xie, 2015. Experiments and parametric studies on 3D metallic auxetic metamaterials with tuneable mechanical properties, Smart Materials and Structures Volume 24, number 9; 095016.

[4] Liu, Q., 2006. Literature Review: Materials with Negative Poisson's Ratios and Potential Applications to Aerospace and Defence, DSTO-GD-0472 (Australian government Defence Science and Technology Organisation).

[5] Evans, K.E. and K. L. Alderson, 2000. Auxetic materials: the positive side of being negative, *Engineering Science and Educational Journal*, pages148-154.

[6] Lakes, R., 1987. Foam structures with a negative Poisson´s ratio, *Science* Volume 235, pages 1038-1041.

[7] Imbalzano, G., S. Linforth., T. D. Ngo, P. V. Lee, and P. Tran, 2018. Blast resistance of auxetic and honeycomb sandwich panels: Comparisons and parametric designs. *Composite Structures*, Volume 183, 242-261.

[8] Imbalzano, G., P. Tran, T. D. Ngo, and P.V. Lee, 2017. Three-dimensional modelling of auxetic sandwhich panels for localised impact resistance, *Journal of Sandwich Structures & Materials*, Volume 19, Issue 3, pages: 291-316.

[9] Naboni, R., and S. S. Pezzi, 2016. Embedding auxetic properties in designing active-bending gridshells, In: *XX Congress of the Iberoamerican Society of Digital Graphics*.

[10] Ai, L., and X.- L. Gao, 2018. Three-dimensional metamaterials with a negative Poisson's ratio and a non-positive coefficient of thermal expansion, *International Journal of Mechanical Sciences* Volume 135, pages 101-113.

[11] Rad, M. S., Y. Prawoto, and Z. Ahmad, 2014. Analytical solution and finite element approach to the 3D re-entrant structures of auxetic materials, *Mechanics of Materials* Volume 74, pages 76-87.

[12] Crespo, J., and F.J. Montáns, 2018. A continuum approach for the large strain finite elements analysis of auxetic materials, *International Journal of Mechanical Sciences* Volume 135, January 2018, pages 441-457.

[13] Crespo, J., M. Latorre, and F.J. Montáns, 2017. WYPIWYG hyperelasticity for isotropic compressible materials, *Computational Mechanics*, Volume 59, Issue 1, pages 73-92.

[14] MSC Software manual, 2012. Marc® 2012, Volume A: Theory and User Information.

[15] MSC Software manual, 2012. Patran 2012, Reference Manual: Part 3: Finite Element Modeling.

[16] Amores, V.J., J.M. Benítez, and F.J. Montáns, 2019. Data-driven, structure-based hyperelastic manifolds: A macro-micro-macro approach. *arXiv preprint*, arXiv: 1903.11545.

[17] Amores, V.J., J.M. Benítez, and F.J. Montáns, 2019. Average-chain behaviour of isotropic incompressible polymers obtained from macroscopic experimental data. A simple structure based WYPiWYG model in Julia language. *Advances in Engineering Software*, Volume 130, pages 41-57.

[18] Romero, X., M. Latorre, F.J. Montáns, 2017. Determination of the WYPiWYG strain energy density of skin through finite element analysis of the experiments on circular specimens. *Finite Elements in Analysis and Design*, Volume 134, pages 1-15.

[19] Crespo, J., F.J. Montáns, 2019. General solution procedures to compute the stored energy density of conservative solids directly from experimental data. *International Journal of Engineering Science*, Volume 141, pages 16-34.

[20] Latorre, M., F.J. Montáns, 2016. The relevance of transverse deformation effects in modeling soft biological tissues. *International Journal of Solids and Structures*, Volume 99, pages 57-70.

[21] Latorre, M., F.J. Montáns, 2015. Material-symmetries congruency in transversely isotropic and orthotropic hyperelastic materials. *European Journal of Mechanics-A/Solids*, Volume 53, pages 99-106.