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**Multi-scale homogenization for 3D multiphase composites:
Development of robust software tools for material/structural
characterization across length scales**

Professor Philippe G. Young (University of Exeter)

**Simpleware Ltd.
Bradninch Hall, Castle Street
Exeter, EX4 3PL, United Kingdom**

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14. ABSTRACT
Synthetic and natural micro-architectures occur frequently and multiphase functionally graded composites are becoming increasingly popular for applications requiring optimized/tailored material properties. When dealing with such materials computationally one issue which immediately arises is the analysis of the mechanical properties of macroscopically inhomogeneous multi-scale structures. The bulk response can be determined by performing full finite element analysis; i.e., with entire geometry discretized at a resolution high enough to model the smallest length scale of interest. However, analyzing these full models may only be possible with the help of supercomputers. Additionally, in an iterative optimization process where performance may be evaluated thousands of times, full FEA simulations become highly impractical. As an alternative, a novel two stage approach to solving such large problem by performing element-by-element homogenization of the micro-structure followed by solving the global problem with a coarser mesh was explored. Results for elasto-statics case showed the approach can provide a viable path from high-resolution 3D imagery through multiscale (two scale) analysis. The approach is now being implemented in code for future release in a version of Simpleware ScanIP, to be applicable for a broad range of physics beyond simply elasto-static loading.

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Principal Investigator: Prof Philippe G. Young, University of Exeter, Exeter, EX4 4QF, UK
Email: philippe.g.young@exeter.ac.uk, Tel: 01392 428750

Researchers: Dr David Raymont and Dr Joonshik Kim supervised by Dr Viet Bui Xuan Simpleware Ltd., Exeter, EX4 3PL, UK

Overview:

A novel approach to solving large multi-scale image based problems was explored opening up the possibility of solving for very large finite element and finite volume problems on modest computational platforms. This is being implemented as a software tool as part of 'Material Toolbox' for use by the research and development community.

Background:

Synthetic and natural micro-architectures occur frequently (e.g. MMC foams, bone, etc.) and multiphase functionally graded composites are becoming increasingly popular for applications requiring optimized/tailored material properties. When dealing with such materials computationally one issue which immediately arises is the analysis of the mechanical properties of macroscopically inhomogeneous multi-scale structures. The bulk response of these structures can be determined by performing 'full' finite element analysis, that is, with the entire geometry discretized at a resolution high enough to accurately model the smallest length scale of interest. However, these full models may easily exceed hundreds of millions, potentially billions, of degrees of freedom and solving problems of this magnitude may only be possible with the use of supercomputing facilities. Additionally, in an iterative optimization process where the 'performance' of the structure may be evaluated thousands of times the use of full FEA simulations becomes highly impractical. When the performance of a structure is evaluated in an optimization process typically only some aspect of the bulk response, such as deflection, is considered. For such properties full FEA simulations model the problem may be excessive. In the present project a novel two stage approach to solving such large problem by performing element by element homogenization of the micro-structure followed by solving the global problem with a coarser mesh as will be outlined below was explored.

Approach explored:

The approach taken is effectively based on creating a coarse tetrahedral/hexahedral discretization of the domain using traditional volume meshing techniques and assigning appropriate material properties based on a finite element homogenization based on high resolution mesh at the micro-structural level of the macro tetrahedra or hexahedra. In effect two length scales are decoupled by computing effective properties using the finite element approach for each macro-element. The novelty here lies in effectively discretizing the 'full' 3D mesh into larger tetrahedra and hexahedra and computing homogenized properties for each macro-element based on exact meshed domains representing the full microstructural complexity within the macro-elements.

Methodology/Project Outline:

The project was implemented in several steps:

1. Homogenization for linear elastic material properties on a hexahedral domain

In the limit of small deformations, elastic materials are described by the linear theory of elasticity. In an elastic body at equilibrium and in the absence of body forces, the stress and strain fields σ and ϵ satisfy the equations

$$\nabla \cdot \boldsymbol{\sigma} = 0, \quad \boldsymbol{\epsilon} = \frac{1}{2} [\nabla \mathbf{u} + (\nabla \mathbf{u})^T], \quad (1)$$

where $\mathbf{u}(\mathbf{x}) := \mathbf{x} - \mathbf{x}_0$ is the displacement of the point \mathbf{x} of the body relative to its position \mathbf{x}_0 in a reference stress-free state [Milton, p. 22]. The rank-two symmetric tensors $\boldsymbol{\sigma}$ and $\boldsymbol{\epsilon}$ are linked by the constitutive relation

$$\boldsymbol{\sigma} = \mathbf{C} \boldsymbol{\epsilon}, \quad (2)$$

where \mathbf{C} is the (rank-four) *constitutive tensor* (also called the *stiffness tensor*; here we avoid this term due to possible confusion with the notion of a *stiffness matrix* used in finite element analysis). In a heterogeneous medium \mathbf{C} is position-dependent [$\mathbf{C} = \mathbf{C}(\mathbf{x})$]. Thanks to this relation, eqs. (1) can be reduced to a single (vectorial) equation for the displacement \mathbf{u} :

$$\nabla \cdot \{ \mathbf{C} [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] \} = 0. \quad (3)$$

In composite media one can usually distinguish three distinct length scales [Milton, p. 7]. The *microscale* is characterized by the typical size l_1 of heterogeneities: it is the scale on which the *intrinsic* material properties, such as $\mathbf{C}(\mathbf{x})$ for elasticity, vary. The *mesoscale* is characterized by a length l_2 at which the material appears “statistically homogeneous”. At this scale constitutive relations, such as eq. (2), become valid *in the sense of averages*:

$$\bar{\boldsymbol{\sigma}}(\mathbf{x}) = \mathbf{C}_{\text{eff}}(\mathbf{x}) \bar{\boldsymbol{\epsilon}}(\mathbf{x}), \quad (4a)$$

where $\mathbf{C}_{\text{eff}}(\mathbf{x})$ is the *effective constitutive tensor* at point \mathbf{x} and the overbar denotes the moving average:

$$\bar{\boldsymbol{\sigma}}(\mathbf{x}) = \int H(\mathbf{y} - \mathbf{x}) \bar{\boldsymbol{\epsilon}}(\mathbf{y}), \quad (4b)$$

where $H(\mathbf{x})$ is some convenient window function, e.g. $H(\mathbf{x}) = 1$ if $|\mathbf{x}| < l_2$ and 0 otherwise.

Finally, the *macroscale* is characterized by a length l_3 at which the *effective* material properties, such as $\mathbf{C}_{\text{eff}}(\mathbf{x})$, undergo substantial variations. If the mesoscale is much smaller than the macroscale ($l_2 \ll l_3$), it becomes possible to radically simplify the conceptual and numerical analysis of the composite medium, while preserving its macroscopic behaviour, by replacing the rapidly varying constitutive tensor $\mathbf{C}(\mathbf{x})$ by the much more slowly varying (or constant) tensor $\mathbf{C}_{\text{eff}}(\mathbf{x})$.

Equation (4) can serve as the operational definition of the effective constitutive tensor \mathbf{C}_{eff} [Hashin 1983]. To calculate its value for a given composite material, one needs then to substitute for $\boldsymbol{\sigma}(\mathbf{x})$ and $\boldsymbol{\epsilon}(\mathbf{x})$ valid solutions of the elasticity equations (1)–(2) in a domain Ω being the support of the window function $H(\mathbf{x})$. The tensor \mathbf{C}_{eff} has 81 components, only 21 of which, however, are independent [Saad 2009, p. 80]. Owing to the symmetry properties of $\boldsymbol{\sigma}$, $\boldsymbol{\epsilon}$ and \mathbf{C}_{eff} it is necessary to use six linearly independent solutions ($\boldsymbol{\sigma}_i(\mathbf{x}), \boldsymbol{\epsilon}_i(\mathbf{x})$) ($i = 1, 2, \dots, 6$) to determine all components of \mathbf{C}_{eff} . In the standard shorthand Voigt notation, in which the stress and strain tensors are written as 6-component column vectors and the constitutive tensor as a 6-by-6 symmetric matrix, the final formula for \mathbf{C}_{eff} is

$$\mathbf{C}_{\text{eff}} = [\boldsymbol{\sigma}_1 \ \boldsymbol{\sigma}_2 \ \boldsymbol{\sigma}_3 \ \boldsymbol{\sigma}_4 \ \boldsymbol{\sigma}_5 \ \boldsymbol{\sigma}_6][\boldsymbol{\epsilon}_1 \ \boldsymbol{\epsilon}_2 \ \boldsymbol{\epsilon}_3 \ \boldsymbol{\epsilon}_4 \ \boldsymbol{\epsilon}_5 \ \boldsymbol{\epsilon}_6]^{-1}, \quad (5)$$

where $\boldsymbol{\sigma}_i$ and $\boldsymbol{\epsilon}_i$ denote column vectors.

Except for composites with very particular geometric structure (for example random ensembles of spherical inclusions), the particular solutions $(\boldsymbol{\sigma}_i(\mathbf{x}), \boldsymbol{\epsilon}_i(\mathbf{x}))$ needed to calculate the effective constitutive tensor must be obtained numerically, and this is the approach we choose. We solve eq. (4) with the finite element method in a hexahedral domain Ω . We use ScanIP to mesh the domain with linear tetrahedral elements and we expand each component of the unknown field $\mathbf{u}(\mathbf{x})$ into globally continuous, piecewise linear scalar basis functions.

The choice of boundary conditions on the surface $\partial\Omega$ of Ω is an important aspect of numerical homogenization. In theory, for a sufficiently large (i.e. statistically homogeneous) domain Ω the same value of the effective constitutive tensor \mathbf{C}_{eff} should be obtained for any field $\mathbf{u}(\mathbf{x})$ satisfying eq. (3) in Ω , and hence for any boundary conditions imposed on $\partial\Omega$. In practice, however, due to limited computational resources, simulations are often done on domains too small to be fully statistically homogeneous. In this case, the imposed boundary conditions do have (some) influence on the calculated values. Four types of boundary conditions are commonly used in literature [Ostoja-Starzewski 2006]:

- kinematic uniform boundary conditions:

$$\mathbf{u}(\mathbf{x}) = \boldsymbol{\epsilon}_0 \cdot \mathbf{x} \quad \text{for } \mathbf{x} \in \partial\Omega,$$

where $\boldsymbol{\epsilon}_0$ is a constant symmetric tensor; it can be shown that $\boldsymbol{\epsilon}_0$ is then the average strain in the domain Ω ;

- static uniform boundary conditions:

$$\boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = \boldsymbol{\sigma}_0 \cdot \mathbf{n}(\mathbf{x}) \quad \text{for } \mathbf{x} \in \partial\Omega,$$

where $\boldsymbol{\sigma}_0$ is a constant symmetric tensor and $\mathbf{n}(\mathbf{x})$ is the unit vector normal to the surface $\partial\Omega$ at \mathbf{x} ; it can be shown that $\boldsymbol{\sigma}_0$ is then the average stress in the domain Ω ;

- periodic boundary conditions:

$$\mathbf{u}(\mathbf{x} + \mathbf{a}_i) = \mathbf{u}(\mathbf{x}) + \boldsymbol{\epsilon}_0 \cdot \mathbf{x}, \quad \boldsymbol{\sigma}(\mathbf{x} + \mathbf{a}_i) \cdot \mathbf{n}(\mathbf{x} + \mathbf{a}_i) = -\boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) \quad \text{for } \mathbf{x} \in \partial\Omega,$$

for \mathbf{a}_i being one of three linearly independent *lattice vectors* $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$;

- mixed orthogonal boundary conditions (for example, uniform strain prescribed on two opposite faces of a cuboid and uniform stress prescribed on the remaining four faces).

In each case, simulations must be done for six linearly independent values of the constant tensors $\boldsymbol{\epsilon}_0$ and $\boldsymbol{\sigma}_0$.

On the boundary $\partial\Omega$, the uniform boundary conditions introduce artificial features that would be absent in a domain Ω situated within a larger body of the composite material. In consequence, simulations performed using kinematic uniform boundary conditions overestimate the effective constitutive tensor [Ostoja-Starzewski 2006], while the application of static uniform boundary conditions leads to an underestimated constitutive tensor. These effects are particularly strong

when the boundary of the simulation domain $\partial\Omega$ intersects material interfaces. Periodic boundary conditions do not have this deficiency, but only as long as they are applied to genuinely periodic composites. Mixed orthogonal boundary conditions are only applicable to materials of orthotropic or higher symmetry [Hazanov and Amieur 1995], and the edges of the hexahedral computational domain Ω must be oriented parallel to the symmetry axes of the material. If these requirements are satisfied, however, mixed orthogonal boundary conditions provide accurate predictions of the effective constitutive tensor already for small computational domains.

Since in general we cannot assume the presence of any particular symmetries in the materials to be homogenized, we have implemented the static and kinematic uniform boundary conditions, which are applicable to all composites and to all shapes of domains Ω .

2. Homogenization for linear elastic material properties on a tetrahedral domain

The homogenization of linear elastic material properties with a regular hexahedral domain, as described in the previous section, is a well-studied topic. However, the class of problems of interest to this project (multi-scale structures with irregular domains) required that a different approach to the calculation of the effective elastic properties be taken. The more straightforward case of a regular hexahedral domain may be addressed by dividing the domain into regular hexahedral elements, each of which can be assigned properties using the classical homogenization techniques described previously.

For the more general case, this work exploited the use of robust all-tetrahedral volume meshing as a method for dividing an irregular domain into smaller sub-volumes for homogenization. As each sub-volume conformed to its parent macro-element a method for calculating their effective properties was developed.

At the highest level the developed homogenization process involves treating the sub-volume as if it were the actual macro-element. Appropriate boundary conditions are applied based on the shape functions of the macro-element such that the sub-volume is constrained to the same modes of deformation. A series of finite element simulations are then performed in order to determine the sub-volume's effective properties. A more detailed description of this process in 2D follows, however the approach taken extends directly to 3D with linear tetrahedral elements.

3. Constitutive Matrix Recovery from a 3 Noded Triangle Element

To highlight the basic principle of the developed homogenization method this section will demonstrate how the material properties of a simple 3-node element can be recovered by way of virtual testing. This in itself has little to no direct practical use, but the principle is fundamental to the developed homogenization method.

The Constant Strain Triangle (CST) element is chosen due to its simplicity.

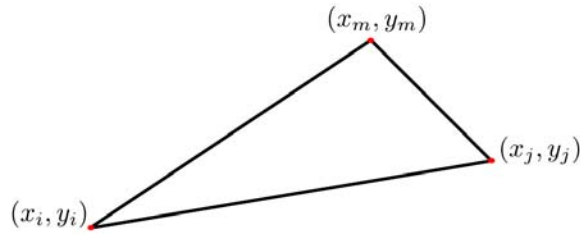


Figure 1: A 3-node constant strain triangle element. Nodes are numbered anticlockwise.

We know that the constitutive matrix and element geometry determine the behavior of the element. This is clear from how the element's stiffness matrix, \mathbf{K} , is calculated:

$$\mathbf{K} = t\mathbf{A}\mathbf{B}^T\mathbf{C}\mathbf{B} \quad (6)$$

where A is the area of the triangle, \mathbf{C} the constitutive tensor and t the thickness of the element. The \mathbf{B} matrix is constructed from the element's shape functions, a set of linear displacement functions. For an isotropic material in 2D the constitutive tensor is defined as:

$$\mathbf{C} = \frac{E}{1-\nu^2} \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{bmatrix} \quad (7)$$

where E is the Young's modulus and ν the Poisson's ratio. Due to symmetry in the matrix there are only six independent components and hence six unknown values to find in the case of general anisotropy.

We know that applying a displacement to one of the element's nodes will result in a force, as described by Hooke's Law:

$$\mathbf{F} = \mathbf{K} \cdot \mathbf{U} \quad (8)$$

where \mathbf{F} is the force vector and \mathbf{U} the displacement vector. Substituting equation 6 into equation 8, it is possible to express these forces in terms of the unknowns, \mathbf{C} :

$$\mathbf{F} = t\mathbf{A}\mathbf{B}^T\mathbf{C}\mathbf{B} \cdot \mathbf{U} \quad (9)$$

The expression in equation 9 will provide a system of linear equations with a set of unknowns. However, for a single test the system is underdetermined and it can be shown that further tests are required to establish an over-determined system. In 2D three tests are required, whereas in 3D six are required. A solution for the over-determined system is then calculated using the least squares method.

Thus far it has been shown that by imposing displacements on the macro element's nodes and measuring the resulting forces it is possible to recover the full constitutive matrix. This alone is of no practical use, but instead provides a starting point for bridging the gap between the micro and macro scale.

In the previous scheme the virtual tests could be described using a simple displacement vector as they were performed on a single element. However, in this case the virtual tests are to be performed on the micro mesh. To achieve this we constrain the displacement of the so-called “external micro nodes” to the surface of the macro element. This constraint is used so that the area discretized by the micro elements is limited to behave as if it were the macro element. To perform the virtual tests we first compute the displacement of each of the external micro nodes. Given a displacement vector

$$\mathbf{U} = \{u_i, v_i, u_j, v_j, u_m, v_m\}$$

we prescribe the external micro nodes displacements using weightings calculated from the macro element’s shape functions, N_i, N_j, N_m :

$$\begin{aligned} \Delta x &= N_i u_i + N_j u_j + N_m u_m \\ \Delta y &= N_i v_i + N_j v_j + N_m v_m \end{aligned} \quad (10)$$

Nodes which do not lie on the macro element’s boundary are left unconstrained.

Following a series of virtual tests a number of forces on the external micro nodes will have been computed. As the process of recovering the effective constitutive matrix requires the forces on the macro element we compute the *effective macro forces* from the *measured micro forces*. Similarly to the calculation of the displacements, the effective macro forces are calculated as a weighted sum of the micro forces using the macro element’s shape function:

$$\mathbf{F}_i = \begin{bmatrix} \sum_{k=1}^n N_i \cdot F_k^X \\ \sum_{k=1}^n N_i \cdot F_k^Y \end{bmatrix} \quad (11)$$

where \mathbf{F}_i is the macro force vector for macro node i , n the number of external micro nodes and F_k^X and F_k^Y the x and y components of the micro force vector for node k . Substituting these effective macro forces into equation 9 we are able to compute the effective constitutive matrix for the sub-volume.

4. Validation:

As part of the validation of the developed homogenization technique for tetrahedral sub-volumes a homogeneous sub-volume with fully anisotropic material properties was used as a “sanity test”. The input material properties were accurately recovered.

More interestingly, the technique was also used to recover the effective properties of a real world structure and compared to the results obtained using classical methods. The Schoen Gyroid was chosen for this purpose as its periodic geometry allows periodic boundary conditions to be used. These boundary conditions are often considered to be the exact solution.

Figures 2 and 3 show the effective Young’s modulus and shear modulus of a sample of the Schoen Gyroid structure at various volume fractions. The effective properties were calculated using the classical homogenization technique with kinematic uniform boundary conditions (“KUBC”), periodic

boundary conditions and with the developed method. In each case a different domain was used to ensure a fair comparison:

- KUBC – a cube of $8 \times 8 \times 8$ unit cells
- Periodic – a single unit cell
- Tetrahedral method – a single regular tetrahedron containing 8^3 unit cells

The results show an excellent agreement between the different methods.

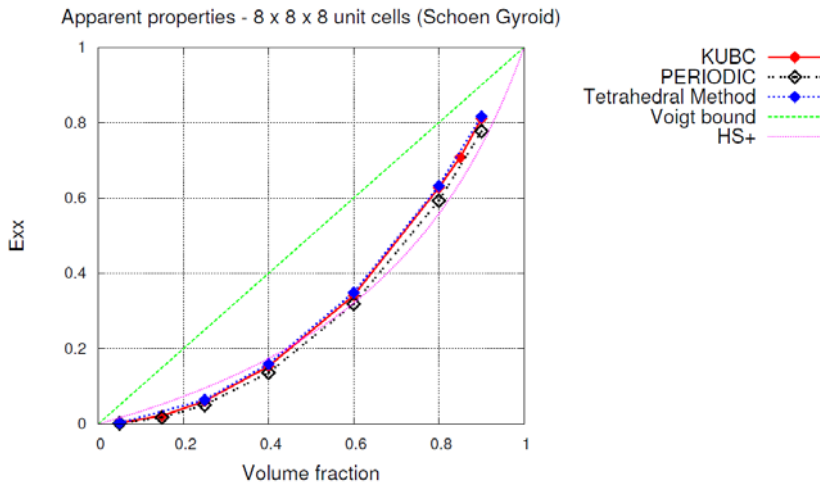


Figure 2: Young’s modulus of the Schoen Gyroid at various volume fractions

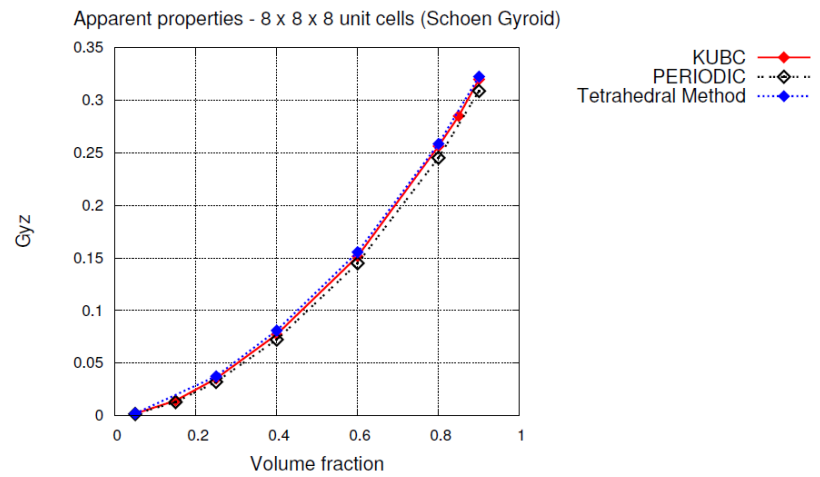


Figure 3: Shear modulus of the Schoen Gyroid at various volume fractions

5. Sequential Solution of Two Stage Problem

Following the development of a technique to determine an effective constitutive matrix for an arbitrary tetrahedral sub-volume we addressed the issue of multi-scale problems. Of particular

interest are the set of problems having an irregular (i.e. non-cuboidal) domain. While problems of a more regular nature may be addressed with more conventional methods of determining effective constitutive matrices, they are never the less addressable using the methods developed in this work.

For many problems it is highly impractical to attempt to include all length scales in a finite element model, consequently it is often desirable to only capture the coarser details. Rather than excluding the smaller length scales we produce a coarse mesh with appropriate homogeneous material properties. The previous section describes the process of computing these properties.

The process of generating the macro mesh is outlined in Figure 4. The homogeneous domain should conform to the bounds of the original domain as closely as possible, representing the result of a 'shrink wrap' operation.

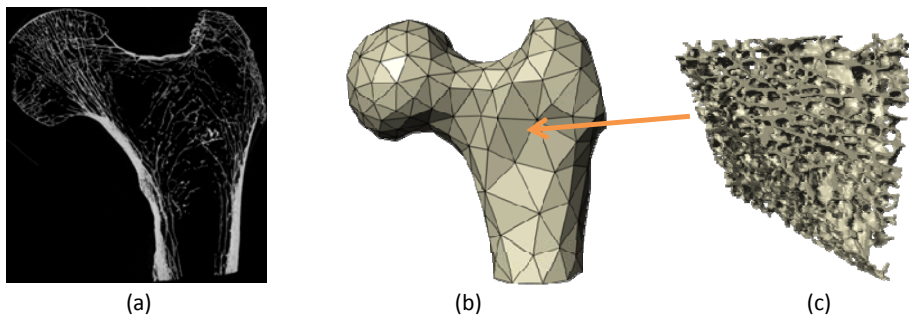


Figure 4: Femoral head modeling (a) input dataset, (b) coarse tetrahedralisation (c) micro-element

Each of the macro elements in the generated mesh is subsequently homogenized using the developed technique. As each macro element is considered as an independent sub-volume the processing may occur in either series or in parallel, depending on the available computational resources. The final result is a macroscopic homogenous model with varying material properties which can be exported to a traditional finite element package.

Conclusions:

Project showed that the approach could be successfully used on problems of interest for the elasto-statics case and a complete pipeline from high resolution 3D image data through to multiscale (two scale) analysis. The approach is currently being implemented in code for release in a version of ScanIP. This is being carried out by Dr Wojciech Śmigaj for a broad range of physics (rather than solely for elasto-statics problems considered under the auspices of EOARDS grant).

Dissemination:

-Invited abstract accepted for oral presentation at Telford-UKIERI workshop on **"Anisotropic, heterogeneous and cellular materials: From microarchitecture to macro-level response"** in Edinburgh, December 12-14th, 2013. See attached abstract.

-Abstract submitted for oral presentation at 2nd International Congress on 3D Materials Science 2014 on **"A novel approach to multiscale homogenisation"** in Annecy, June 29th - July 2nd, 2014.

-Abstract submitted for oral presentation at 11th World Congress on Computational Mechanics (WCCM XI) on “**A novel approach to multiscale homogenisation for 3D micro-structures**” in Barcelona, July 20-25th, 2014.

-Paper in preparation on “Multi-scale homogenisation”

-Visit to be arranged to AFRL Dayton, Ohio to present work carried out and explore collaboration with AFRL research staff

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