Conference Presentation

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McMillan, A.

This is a paper presented at the *Advanced Materials for Demanding Applications conference*, 7-9 April 2014.

Recommended citation:

McMillan, A, (2015), "Geometry generation challenges for modelling and analysis of micro-structured materials", in *IOP Conf. Series: Materials Science and Engineering*, Vol.74, 012010. *Proceedings of Advanced Materials for Demanding Applications conference*, 7-9 April 2014, St. Asaph, UK. doi: 10.1088/1757-899X/74/1/012010

Geometry generation challenges for modelling and analysis of micro-structured materials

AJ McMillan

Professor in Aerospace Technology, *Glyndwr University*,
Mold Road, Wrexham, LL11 2AW, UK.

a.mcmillan@glyndwr.ac.uk

Abstract. Engineers evaluating the performance of a component at the design stage will typically convert Computer Aided Design (CAD) geometry into a Finite Element model, and run a Finite Element Analysis (FEA) to determine deformations and stress levels as a result of applied loads or displacements. The analysis results would then be interpreted by comparing them with the required duty of the component. For metallic components, homogeneous and isotropic material properties are generally assumed – "macro-scale" modelling. For components to be manufactured from composite materials, models may represent heterogeneity at the ply level, and orthotropic material properties applied with appropriate directionality. This ply-level modelling is often termed "meso-scale" modelling. Engineering interpretation of failure in materials is often based on empirical understanding of experimental data. This approach is generally robust: safety critical components would always be subject to validation by means of a suitable programme of testing. The aspect that is missing is the opportunity to improve understanding of the material performance by investigating the material performance at the "micro-scale". This paper describes computational algorithms for generating random geometries exhibiting similar characteristics to those seen at the "micro-scale" in real materials, and the use of these to predict the influence of the "micro-scale" structure on the "macro-scale" material performance.

1. Introduction

Almost all materials exhibit some heterogeneity at some length scale: for example, the crystal grain structure in metals, or the individual filaments of fibre in a fibre reinforced composite. Such details are known to play a role in the material performance: for example the strength and ductility of a metal is highly influenced by the crystal grain size and configuration.

The purpose of this paper is to describe the modelling challenges presented by the representation of the micro-structural heterogeneity, and to present results that display remarkable or unexpected details. The mechanical analysis technique adopted here is finite element method [1]. For example, the lower right hand image in Figure 1 illustrates the formation of stress banding in a material containing randomly arranged holes [2].

2. Brief literature review on geometry generation

Geometry creation seems to be a melting pot of disciplines, with relevant literature to be found not only in journals of engineering and applied mathematics, but also in text books and web guides for computer generated art and computer games [3, 4, 5].

Within the engineering literature, much of the geometry creation work is largely focussed on the modelling of fibre and resin geometry within composites. [6, 7]. Methods of modelling uncertainties in geometry, for example to represent the influence of design tolerance allowables on component strength, are at an early stage of development [8, 9, 10], but the modelling of random features or flaws does not seem yet to have been systematically studied.

3. Porosity in materials

Material porosity is a particular issue for many manufacturing processes, because it is known, for example [11], that porosity reduces the strength of the manufactured component. If a material has holes in it, does it make it weaker, and if so, by how much? Although this seems to be a very simple question, it is rather difficult to specify in a way that can be answered in a quantifiable manner concerning the strength of the component.

On a production line, a manufactured part exhibiting more than a prescribed percentage of porosity will be scrapped. In general, the actual porosity is not measured directly – a direct and accurate measurement system would not be cost effective. In a similar way, the strength reduction resulting from a given level of porosity is not measured in the as manufactured component, but arrived at from previous experience. It would seem that better understanding of the influence of manufacturing process variables and the particular component geometry could lead to a more predictive understanding of what would constitute an unacceptable level of porosity.

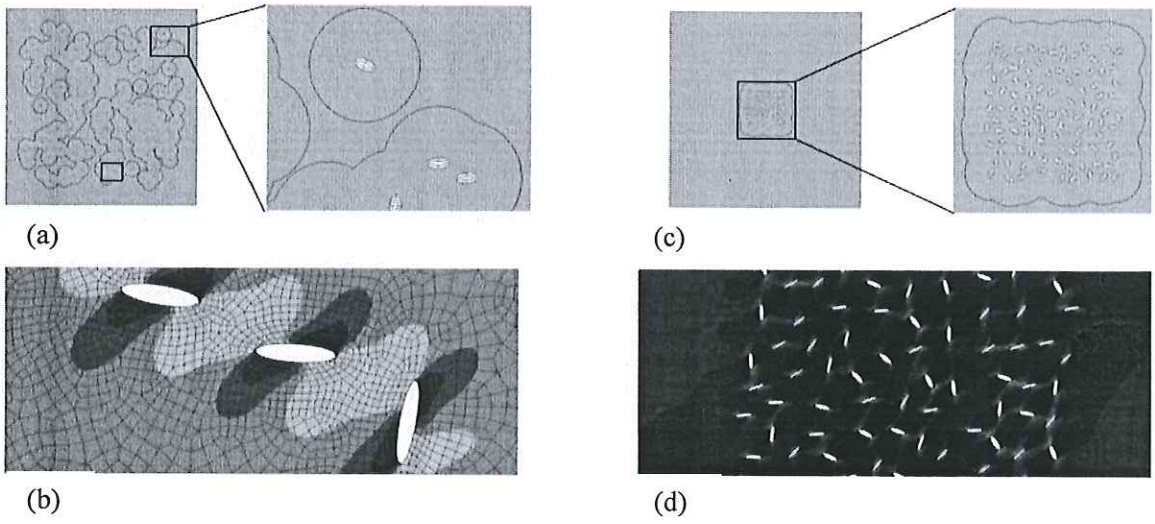

Figure 1. A material filled with elliptical holes; loose packing (a, b) and closely spaced (c, d). The upper Figures (a, c) show the two model domains. The mesh quality is controlled automatically using multiple partitions, indicated by the grey lines; and the yellow regions indicate regions of identical mesh configuration. Figure (b) shows the resulting stress pattern in the vicinity of the three particularly closely spaced holes indicated by the blue rectangle in (a), with the mid blue representing the nominal stress. In (c, d) the packing arrangement is much tighter, but the stress levels (d) are not particularly increased because all the holes are a similar distance from each other. Here the boundary between blue and black regions represents the nominal stress. The stress pattern forms bands and the holes tend to shield each other from extreme stresses.

The model presented in Figure 1 represents a very simplistic initial investigation [2]. A square of material was modelled with Abaqus finite element software, and filled with elliptical holes placed at random but prevented from touching or overlapping. This process was automated using a Python

script to create geometry, ensure the proximity conditions, and then generate the finite element mesh and initiate the analysis. The construction curves shown in the pink diagrams help to define and control the topology of the finite element mesh. The square was then subjected to a shearing load to simulate a realistic stress state. In this initial study two forms of packing were defined.

A conclusion from this particular study was that maximum stress increases very slowly with the number of holes, so long as the holes are distributed in a homogeneously random manner. The strength reduction calculation was based on maximum stress values, but control of the mesh around the region of the hole was essential, to ensure against mesh influence [2]. Since the geometry generation algorithm has a major influence on the result, a study of random geometrical forms and a means for categorising them is essential for further development of this field.

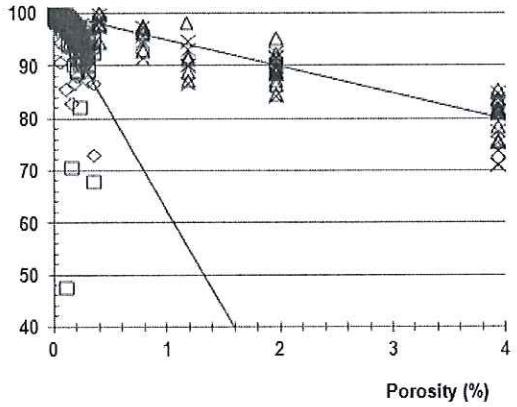

Figure 2. This graph indicates the percentage strength reduction as a result of percentage porosity. There are two distinct sets of data: the essential difference is that where the proximity between pores is more carefully controlled (blue triangles and crosses) a much higher porosity level can be tolerated than in the case where the porosity was more random (red rectangles and diamonds). Note that the red best fit line has been extended beyond the region of applicability, in order for it to be visible.

4. Modelling materials with quantified heterogeneity

Following the initial study, it became clear that a material modelling capability was needed that provided a measurable level of "heterogeneity". Finding an appropriate measure for heterogeneity is a significant part of the problem; nevertheless this has the potential to reveal physical understanding of phenomena that until now have been modelled on the basis of empirical observation.

To put this into context, until now, in component stress analysis, engineers have been obliged to assume material homogeneity, and to adopt pragmatic models for such phenomena as plastic flow, fracture mechanics, and creep. Developing a modelling methodology that can represent a more realistic level of heterogeneity is the starting point to discovering a physical basis for many of the material behaviour rules that are currently determined empirically, and characterised by test.

Ideally, results obtained this way should change the engineering perspective on materials characterisation, but this represents a major undertaking. The obvious challenge is to create the methodology: the less obvious, but potentially far greater, challenge is to persuade the engineering fraternity that such an approach is credible and has the potential to reduce testing costs and lead to better understanding of material performance.

4.1. Empirical vs. real-physics model geometry creation

The challenge is to create realistic geometry for the representation of heterogeneous materials. There are three fundamentally different approaches to generate such geometry. The direct approach is to take a real physical artefact, and generate geometry by measurement. The development of CT imaging capability and the image processing tools means that this is now a genuinely feasible approach [12].

Alternatively, geometry can be created empirically, using CAD drawing tools and lots of imagination. There are two major difficulties here: firstly finding a methodology that can produce realistic looking geometry automatically, and secondly having a algorithmic method for characterizing and validating the "empirical" geometry in comparison with "real" geometry.

A third method is to make use of software embodying relevant physical models, and use the software to develop the model. For example, in Abaqus, a set of hollow spheres could be created, either as elastic solids, or more simply as rigid surfaces, with appropriate contact rules. These could be modelled falling into a box. The physics of contact and mass under gravitational load would ensure that the spheres pack in a realistic way, where the sides of the box arranged to avoid the possibility of perfect packing. Geometry tools could then be used to form a solid, with the insides of the sphere representing the porosity.

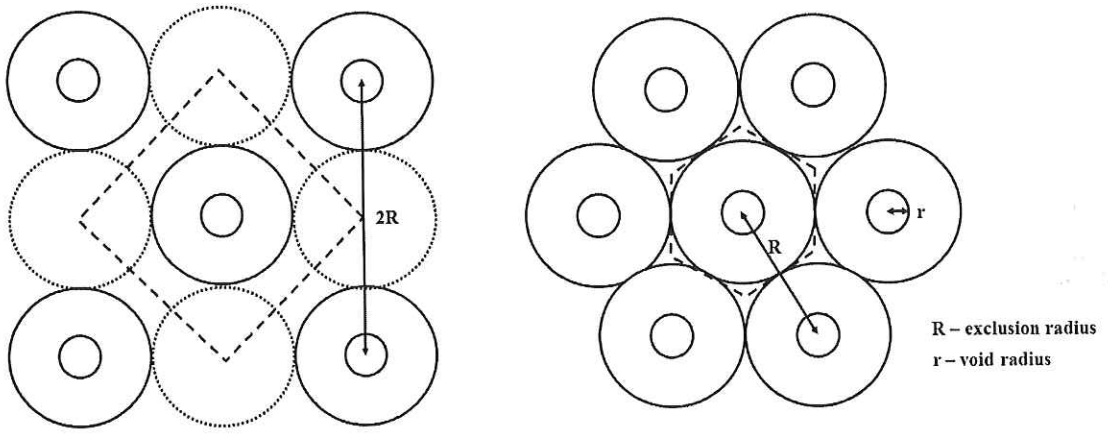

Figure 3. 2D Poisson disc minimum and maximum packing configurations, respectively.

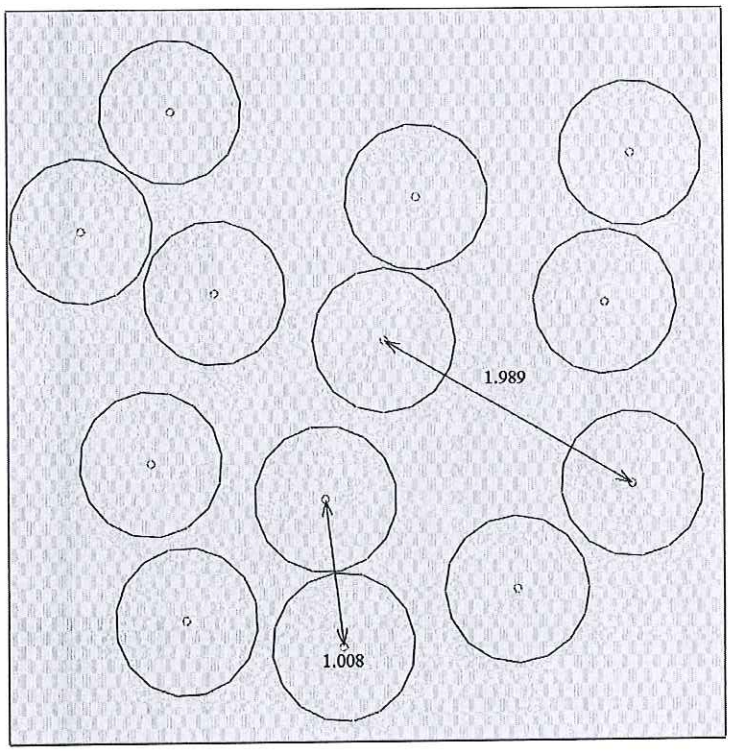

Figure 4. A random porosity model generated in Abaqus using Python. Notice that, even for a small number of seed points, it is not possible to predetermine the number necessary to obtain a "fully dense" packing. The measurements given in this figure demonstrate that the sparse regions are indeed too small to accommodate an additional seed, and the fully dense packing can be verified by inspection.

4.2. Modelling porosity

Currently, the approach adopted here is to generate 2D geometries using empirical methods. A random number generator is used to define "seed" points throughout the domain, onto which geometrical features are then built. The distribution of the seed points [13, 14] is controlled using the Poisson disc method [5].

The Poisson disc exclusion principal is illustrated in Figure 3. The two configurations represent minimum and maximum packing densities, subject to a rule that no seed point can be closer to another than by an amount R, and that every available space is filled – "fully dense packing". Figure 4 shows a typical result of a Python implementation of a Poisson disc algorithm in Abaqus.

For larger numbers of seed points this scheme is no longer feasible. This is a convenient point at which to introduce the notion of "partial packing". This may be quantified in terms of the ratio of actual seeds placed to the number of seeds required for either the theoretical maximum or minimum fully dense packing. To illustrate this, Figure 5 shows four different packing configurations, each representing the same number of seeds but for different values of R. In this case, the seed points define the centres of small pores in a material, and a nominal biaxial stress field has been applied creating a shearing deformation. The colours indicate relative stress levels [14].

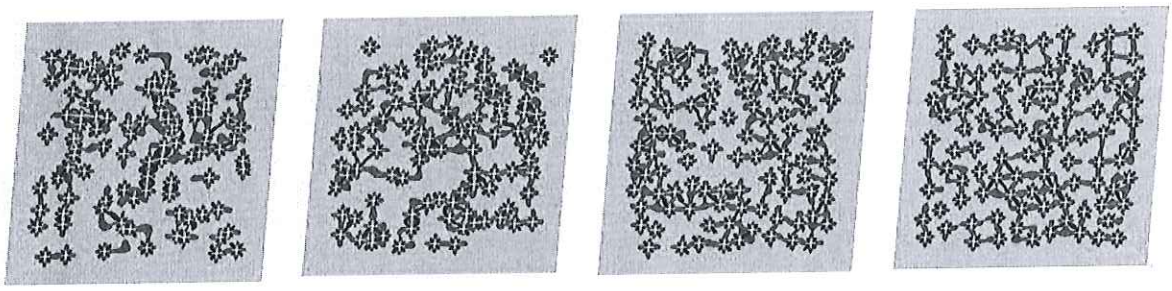

Figure 5. Stress distribution in four models with identical porosity, but with increasingly homogeneous distribution from left to right. Notice how the stress pattern distribution becomes more homogeneous as the seed point distribution tends towards fully dense.

5. Modelling crack propagation in porosity clusters

While single crack propagation using Abaqus XFEM is now a well-established capability [15, 16], multiple crack growth in a porosity cluster is yet to be understood.

Here a problem domain is defined as illustrated in Figure 6. A Python script is written to generate the geometry and partitioning, to enable automatic meshing. Unit traction loads are applied at the boundary to create a biaxial stress state with principal stresses aligned to the diagonals.

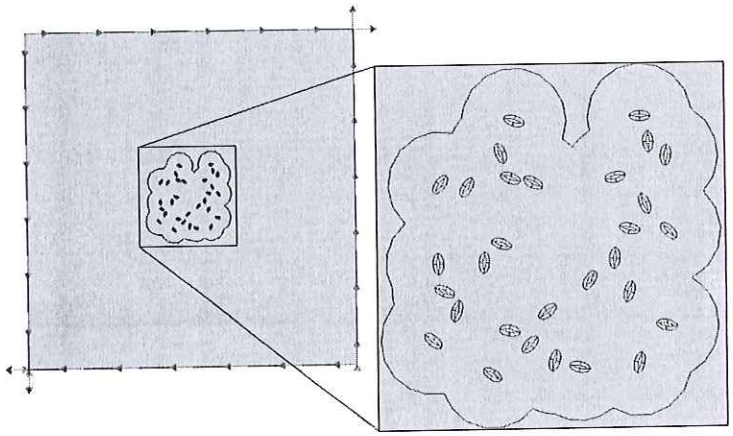

Figure 6. A 2D square of resin material, with a central cluster of randomly positioned elliptical voids.

In Abaqus analysis the loads are ramped up until conditions to initiate cracks are met. Stress levels in some regions are similarly high, and while XFEM is a powerful tool, some care must be taken to ensure all relevant cracks are initiated. XFEM analysis is based on a mesh free enrichment of the domain in the region of the developing crack, and is therefore mesh independent. At each increment, the domain around the propagating crack is re-meshed, nevertheless varying the mesh is sufficient to highlight a problem with sensitivity of crack initiation condition threshold (Figure 7), and raises a question regarding mesh dependency. While such small modifications might influence actual crack path, taken on balance, do the cracks modelled resemble reality?

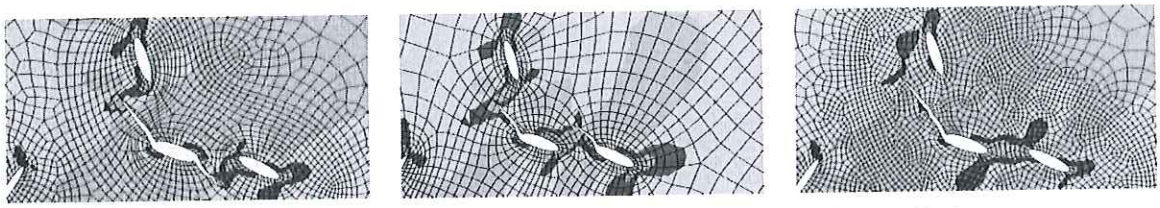

Figure 7. Mesh sensitivity in crack initiation and propagation prediction.

6. Modelling heterogeneous polycrystalline materials

In modelling polycrystalline material structure the same seed point approach can be used. For example, this may mimic the seeding of crystal formation in the solidification of a metal. Again a Poisson disc algorithm can be used to provide a quantified level of "heterogeneity". The challenge here is to find a method for generating realistic crystal boundaries.

While the solidification seed point of the crystal can be modelled by the Poisson disc random seed point together with a random crystal orientation, the individual crystal boundaries could be defined by Voronoi tessellation based on the set of seed points. Thus each Voronoi cell represents a single crystal with randomly prescribed orientation.

This is equivalent to assuming that each crystal in a domain of material starts to solidify at the same time, at the same rate, and isotropically. In reality, different regions of material in a casting mould will cool at different rates, and crystal growth would be anisotropic, influenced by temperature gradient, crystal orientation, and crystal species.

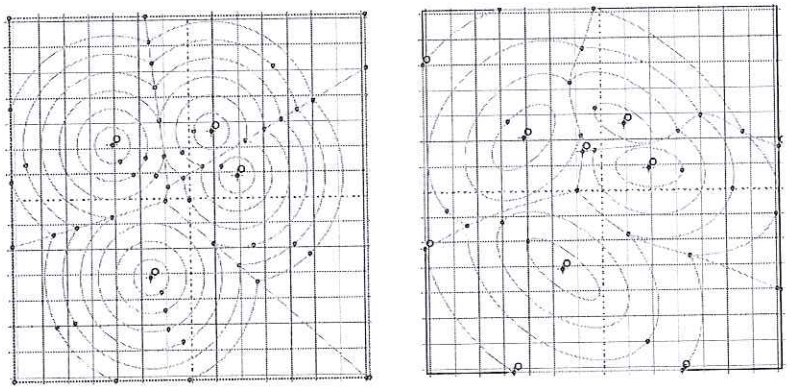

Figure 8. Voronoi tessellation (left) and a modified tessellation for anisotropic boundary growth and time varying growth rate (right). Notice that in this case, the boundaries between crystals are not straight lines.

The most efficient method of creating a Voronoi tessellation is Fortune's algorithm [3, 17], but Figure 8 illustrates a growth based method.

7. Direct modelling of elastic wave propagation

As an alternative to direct geometrical modelling and interpretation of measured geometry, it is possible that the physics of elastic wave propagation through a porous or heterogeneous material could provide results which could be interpreted to provide a measure for porosity or heterogeneity.

Explicit Finite Element is capable of capturing dynamic events, where the elastic wave frequency that can be modelled is limited by the element size, which must be an order of magnitude smaller than the wavelength of vibration.

Thus, by choosing appropriate element sizes and making appropriate modelling choices, it is possible to verify the classical mathematical predictions of wave propagation [18], or to run an analysis on a structure with appropriate initial conditions to ensure vibration is initiated, but with sufficient duration that the standing waves form (Figure 9).

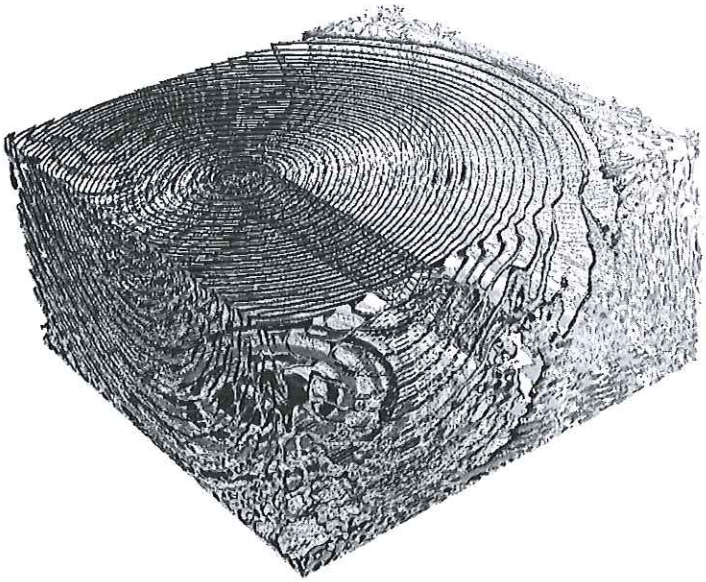

Figure 9. A simulation of high frequency elastic wave propagation, with wave deformation visualised on the external surfaces of a solid block with a central cylindrical hole [19].

In principle, a modelling process such as this could be used to simulate ultrasound based Non-Destructive Test results. Used in tandem with shape optimisation methods, this could provide a technique for enhanced interpretation of results for improved prediction and quantification of flaw size, distribution and location.

8. Discussion – going beyond the current finite element formulation…

In addition to the geometry and modelling challenges presented above, there are two further areas which are worthy of particular consideration.

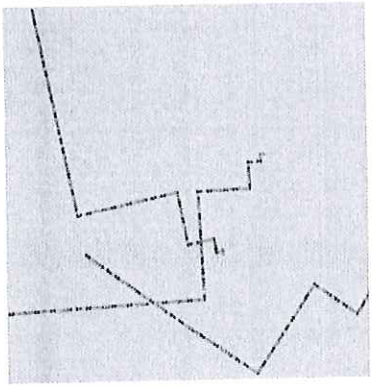

Figure 10. This figure was constructed in Abaqus, using Python, and identifies a fractal path comprised of incremental particular coordinate points within an analysis model. Following analysis, these particular points could be interrogated, taking significantly less time than a review of a full 3D search of the solution domain.

8.1. *Post-processing –searching and manipulating analysis output data*
Routine linear elastic time-independent analysis of homogeneous material domains provides analysis results in which the stress maxima are conveniently located on the surface of the component. As analyses become more sophisticated, it becomes rather more difficult to establish which results are critical and should be assessed. The idea illustrated in Figure 10 is to use 1D fractal based search paths to explore the 3D results domain [14, 20, 21].

8.2. *Solvers which reflect geometrical uncertainty*
In addition to the assumption of material homogeneity, engineering component stress analysis is invariably based on as-designed, or minimum tolerance geometry, but where an as manufactured high value component departs from design allowables it can be time consuming for it to be re-analysed.

Radically different computational solvers might present an alternative approach to standard finite element method, with approaches such as sub-structuring, Mesh-free methods and XFEM already main-stream, but other formulations could provide the key to fast geometry update and re-analysis, as well as critical stress location identification [22].

9. Conclusions
This paper presents a range of challenges presented by materials with heterogeneous properties at the micro-scale. There are a number of open questions for which the development of better computational geometry creation capability would provide useful functionality. Particular lessons already learned are that the length-scales of heterogeneous features, and their orientation and distribution, will have an impact on the macroscopic material properties. It is likely that improved representation of microscopic features could lead to a phenomenological understanding of material behaviours, such as fracture mechanics and creep, which are currently modelled on a macroscopic empirical basis.

Acknowledgements
The initial part of this work was supported under a Royal Society Industry Fellowship.

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