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Virtual testing of advanced composites, cellular materials and biomaterials: a review

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Abstract

This paper documents the emergence of virtual testing frameworks for prediction of the constitutive responses of engineering materials. A detailed study is presented, of the philosophy underpinning virtual testing schemes: highlighting the structure, challenges and opportunities posed by a virtual testing strategy compared with traditional laboratory experiments. The virtual testing process has been discussed from atomistic to macrostructural lengthscales of analyses. Several implementations of virtual testing frameworks for diverse categories of materials are also presented, with particular emphasis on composites, cellular materials and biomaterials (collectively described as heterogeneous systems, in this context). The robustness of virtual frameworks for prediction of the constitutive behaviour of these materials is discussed. The paper also considers the current thinking on developing virtual laboratories in relation to availability of computational resources as well as the development of multi-scale material model algorithms. In conclusion, the paper highlights the challenges facing developments of future virtual testing frameworks. This review represents a comprehensive documentation of the state of knowledge on virtual testing from microscale to macroscale length scales for heterogeneous materials across constitutive responses from elastic to damage regimes.

Keywords: A. Polymer-matrix composites (PMCs); C. Computational modelling; C. Numerical analysis; E. Weaving; Virtual Testing.

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1.0 INTRODUCTION

The need to advance the understanding of the mechanics of many engineering materials has led to developments of analytical, computational and phenomenological methods for predicting the behaviour of such materials. About ten years ago, Oden and co-workers [1] predicted that virtual design, in other words virtual testing, will be one of the key areas that will revolutionize computational mechanics research. According to the authors, this will require development of "*radically new computational tools, with the ability to handle multiscale phenomena, very heterogeneous materials, and discontinuous behaviour, such as fracture and assessment of the range of performance…*" [1]. As the authors predicted, in the last decade, the use of virtual testing methods as predictive tools for understanding the mechanics of engineering materials has become commonplace. Firstly this is encouraged by better understanding of the physics of microscale response of materials. Secondly, the improvements in computational powers have encouraged researchers to begin modelling a wide range of mechanical responses originating from atomic [2] and microscale length scales which serve as inputs for predicting constitutive behaviour at the structural level [3-6]. Therefore such developments have resulted in various forms of virtual laboratories that could eventually become substitutes to physical experiments under certain conditions [7]. Typical examples of *virtual experiments* [2, 5, 6] are described by the originating authors using various keywords as: c*omputational experiments* [8]*, virtual laboratories* [9], *numerical testing machines* [7], *virtual frameworks* [10, 11], *immersive virtual environments* [12]*, in-silico experiments* [13], etc. In the context of this work, the authors will make interchangeable use of any of the following terms to refer to a virtual testing framework: *virtual laboratory, virtual testbed,* and *virtual framework.*

The main driving factor towards the use of advanced materials for structural applications in engineering, healthcare, sports equipment manufacture industry, etc is the possibility of engineering novel materials by altering the microstructural composition. According to Jones and Ashby [14], the possibility of developing novel and improved materials is the *underpinning technology which can stimulate innovation in all branches of engineering.* Advances in understanding of the physics of materials and improvements in computational capabilities have led to development of niche heterogeneous materials described as *tailored or designer* or *smart materials* [15]. These materials possess a combination of mechanical properties that can be adapted (by altering their microstructural composition) to make them suitable for different design requirements. The microstructural adaptation in some cases involves molecule-by-molecule assembly of their constituents [16, 17]. The science of microstructural modifications has also led to development of many different categories of high performance materials like textile composites, functionally graded materials, 3D reinforced composites, tissue-engineering enhanced biomaterials, nano-composites, etc. For the purposes of this paper, all these advanced materials are broadly described as *heterogeneous systems*. The enhanced

properties arise from the possibility of altering their multi-component microstructural compositions. However, this advantage also presents the predictive modelling challenge they pose to material modellers.

Research in virtual testing of heterogeneous materials is still relatively limited and to date there has been no structured compilation of the current state of knowledge. However, such information is necessary as a growing community of researchers are working on virtual testing of continuous fibre reinforced composites [3, 18]. This paper aims to present a detailed review of the existing virtual testing approaches for a wide class of heterogeneous materials namely: composites, cellular materials and biomaterials. This is by no means an exhaustive list as other possible heterogeneous materials include: functionally graded materials, piezoelectric materials, etc. The paper also documents the challenges facing developers of virtual testing frameworks in order to make such methods realistic substitutes for physical experiments. Emphasis is on recent literature of virtual testing of heterogeneous materials; published in the last decade.

The term *virtual testing* is commonly used in aerospace industry to describe the extrapolation of coupon-level experimental data towards understanding the fracture mechanics of structural parts of the aircraft [19, 20]. The aircraft industry uses virtual testing as a design tool thereby reducing the cost of expensive structural testing of new aircraft variants which can cost as much as $40 million [5]. Whilst such application of virtual testing theory is laudable and widespread, the scope of this review article does not encompass such structural level applications of virtual testing. The strategy of using coupon-level data for predicting structural response falls outside the scope of this paper. Rather this work deals with relevant literature on the application of virtual testing of heterogeneous materials by tracking the effect of microstructural modifications on macroscale predictions.

The paper first presents an *overview of virtual testing* before discussing the *roles of lengthscale in designing virtual experiments*. The *structure of typical virtual testing laboratories* is also presented and typical examples considered. Subsequently, the paper describes different *virtual testing implementations for a wide class of heterogeneous materials***,** ranging from composites to biomaterials. Finally, the paper concludes with delineating the *challenges facing the development of new virtual testing frameworks***.**

2.0 VIRTUAL TESTING: AN OVERVIEW

Over the last two decades, virtual testing of heterogeneous materials has been generally accomplished by numerical modelling tools after the finite element method (FEM) [10,12,13]. Although the research investigation for virtual tests differs considerably from case to case, there are, however, several distinct steps typified by these strategies, necessary to execute a virtual test. Firstly, the virtual problem domain of interest must be defined: this involves developing a geometry/domain

that represents the material to be investigated, or, defining a boundary within which the *virtual matter* of interest exists. Secondly, the constitutive behaviour of the declared virtual domain must be defined; for example, the material may exhibit a classical Hookean behaviour or a pre-defined non-linear constitutive behaviour, etc. Thirdly, boundary conditions must be imposed on this domain: this may be in the form of body forces, displacements or thermo-mechanical loading, etc. Fourthly, the constitutive response (i.e. stress-strain curves) of the virtual domain is obtained either directly or through appropriate homogenization techniques. The final, important step in the virtual testing framework is a *validation exercise* which involves comparing the constitutive response(s) obtained from the virtual tests with available experimental or analytical data.

Although the foregoing outlines the basic steps involved in performing virtual tests; in reality, several issues exists that present considerable challenges. The mechanical behaviour of any material is a consequence of synergistic combination of its constituents (i.e. atoms, crystals, crystal planes etc.). For heterogeneous materials, this is particularly true because of the relationship that exists between its constituents (i.e. in composites the matrix and fibres) as well as the internal structure of its individual constituents (i.e. atomic structure of fibre or matrix etc.). Thus, the features that are responsible for the behaviour of heterogeneous materials exist across several domains, spanning a spectra of length and time scales. There arises therefore the challenge of incorporating the physics behind each relevant feature, at each relevant length and time scale, which affects the constitutive behaviour of the virtual domain of interest. The next section considers the place of length scale in virtual testing, and in later sections different variants of virtual testing frameworks are considered.

3.0 VIRTUAL TESTING AND LENGTH SCALES

The determination of a relevant length scale is central to computation of properties of heterogeneous materials. Rudd and Broughton [21] stated that the central aim of computational materials physics is the accurate description of specific materials on length scales spanning the electronic to the macroscopic. Heterogeneity in these *designer materials* suggests that there will be microscale constituents whose composition, orientation and evolution influence macroscale properties. Therefore, at the onset, it is important that length scales be defined for common heterogeneous materials with a view towards understanding the development of virtual tests for such materials.

Typical length scales for describing the response of engineering materials range from atomic/molecular to structural lengthscales. At the atomic length scale, a typical length dimension, L is very much less than 10^{-9} m; whilst at the nanoscale, the length dimension is in order of a nanometre. The microscale is usually in orders of magnitude of a micron, while the mesoscale is a

couple of millimetres. The macroscale is in dimensions of centimetres and structural lengthscales are in orders of meters. **Figure 1** shows the order of increasing lengthscales and the applicable area of computational experiments where each length scale can be used.

Current virtual testing research is based either on a bottom-up (hierarchical) or top-down (concurrent) modelling implementation. The bottom-up implementation determines constitutive behaviour of the heterogeneous material by building up a detailed understanding of the material's constitutive behaviour, from lower length scales through to higher length scales, by utilizing robust constitutive models of the constituents of the test material [22-24]. In the lower length scale regime, lower order behaviour can include crystal plasticity [25], macro-molecular mechanics [26, 27], fibre rupture/kinking and matrix cracking in composites [28], bone tissue porosity [24], cell walls distortions in cellular materials [29], fibrillar and molecular deformation mechanisms of collagens[30], fibroblasts and tenocytes mechanics [31], etc.

Regarding the bottom-up approach, the differences in lengthscales present a challenge towards relating the predictions at lower scale to macroscale/structural level validation data. Bottom-up modelling schemes generally focus exclusively on a distinctly resolved length scale, beginning at a lower order length scale. However, in modelling phenomena at a higher length scale (i.e. length scale higher than the one considered during the initial analysis), homogenizations are invoked in order to harmonize constitutive responses on both length scales. This approach may be computationally efficient, compared to the other approaches. However, certain important microstructural information is suppressed during homogenizations resulting in predictions made at a higher length scale diverging from actual responses.

On the other hand, the top-down approach *"focuses on engineering necessity"* [32]. In essence, this approach requires identifying a constitutive law of a micro-component from a macroscopic test; this involves using higher length scale information to predict lower length scale response. Many phenomenological approaches fall under the top-down approach and such approaches can be quite useful in an industrial environment especially when further refinements are made to the initial model.

Multiscale computational modelling uses the principle of prediction across various lengthscales, often referred to as hybrid lengthscales [9]. Raghavan and Ghosh [33] used a concurrent multiscale analysis in virtual testing of a metallic composite material. Their model bridged three lengthscales namely (a) macroscopic domain (level – 0), (b) macro-micro domain (level-1) with the micro-domain represented by the periodic repetition of a representative volume element (RVE) and (c) microscopic domain (level-2) where the RVE ceases to exist and sub-microstructural features need

to be modelled adequately. For a virtual testing framework, it is essential that the question of appropriate lengthscale and modelling philosophy has to be addressed right at the onset.

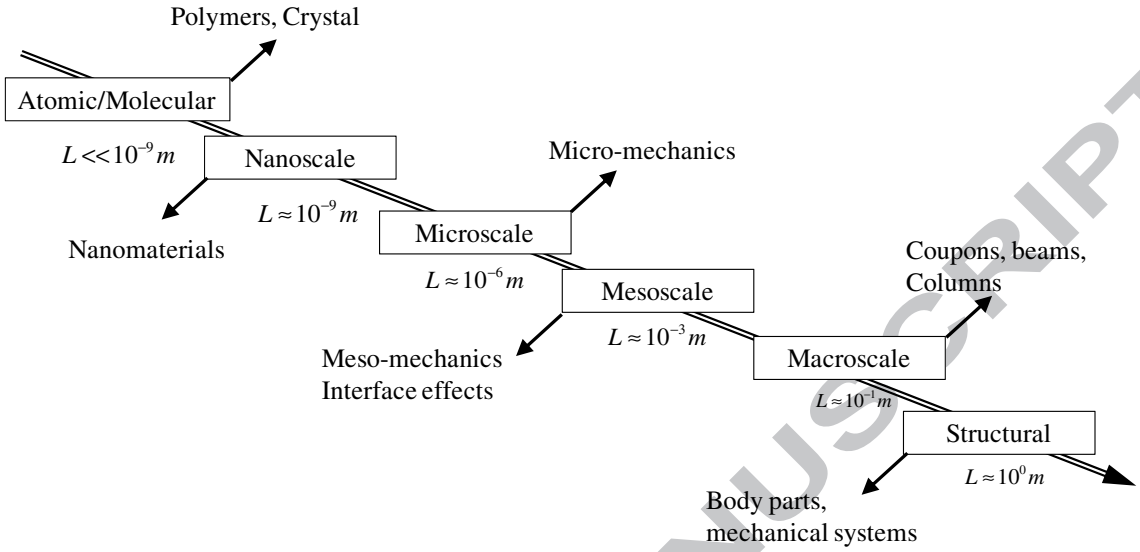


Figure 1: Typical lengthscales used in computational materials science. The different scales are shown in order on increasing dimensions.

4.0 VIRTUAL TESTING OF HETEROGENEOUS SYSTEMS

This section presents a review of virtual testing for different classes of heterogeneous materials. The discussion presents the current implementations highlighting their pros and cons.

4.1 Composite Materials

Composite materials are the most widely tested material using virtual testing schemes [3]. The use of numerical modelling approaches towards investigation of the constitutive behaviour of composites has proved very useful in dealing with the effect of the complex microstructure of composite materials on their structural level response. According to Gonzalez *et al* [3, 34], composites materials are a *paradigm* of virtual testing since the prediction of their effective properties depend on volume fraction, spatial distribution of inclusions and properties of phases and interfaces – all features that can be modelled reliably within a numerical environment. Five classes of composite materials are discussed in the following sections

4.1.1 Unidirectional (UD) Continuous Fibre Composites

The use of virtual testing in modelling of unidirectional continuous fibre composites is widespread. Some of the authors who have developed virtual testing techniques for UD composites include: Cox and Yang [32], Gonzalez *et al* [3], Hallet, *et al* [35], Zhang *et al* [8], Llorca, *et al* [36],

Mikulik, *et al* [4], Irisarri, *et al* [37], Okereke and Akpoyomare [11], etc. Most of the publications considered here are within the last seven years. The application of virtual tests in unidirectional composites, as documented in these publications is mainly to assess elastic, fracture and damage properties of UD composites.

Cox and Yang [32] published one of the earliest review papers on virtual testing of structural composites. In this work, the authors assessed the suitability of existing material models for use in fracture modelling of unidirectional composite materials. The work considered the implications of using different modelling techniques to perform virtual fracture testing; they considered several cohesive zone models (e.g. hybrid stress-strain and traction-displacement models). The authors hypothesized that the expectation of virtual testing as replacement of physical experiments is realistic. Following this initial Cox-Yang paper, Gonzalez and co-workers [3] demonstrated the use of virtual fracture tests in computing the evolution of fracture toughness of SiC fibre-reinforced Ti-matrix composite as a function of temperature. Notched panels were subjected to three-point bending, and finite element simulations were used to model the mechanical response. In the end, the authors obtained quantitative values of fracture resistance of UD composites. The simulations reproduced not only the *micro-mechanisms of deformation and fracture* in the composite material but also provided *quantitative* results of the fracture of composites: thus validating the objective of using virtual fracture tests in place of physical experiments.

Hallet *et al* [35] carried out a numerical analysis of open-hole tensile test of a UD composite. Open-hole tensile tests are used to determine open-hole strength of materials: a useful parameter in calculating the allowable stress in composite design. The results from experimental open-hole tensile tests are significantly affected by factors such as as: composite layup/configuration, hole-size effect, etc which consequently make it difficult for modellers in determining the open-hole tensile strength. The authors therefore used a virtual testing approach to investigate this problem and independently assessed the effects on open-hole tensile strength of: *thickness scaling regime, absolute thickness, in-plane dimensions, stacking sequence, layup and specimen width-to-hole diameter ratio.* The authors established that this approach should provide significant insight into effects of sub-critical damage to ultimate failure of UD composites. The work serves to justify again the use of virtual testing as an increasingly popular tool for understanding the effect of microstructural mechanisms (in this case sub-critical damage) on the macroscale/structural response of the composite.

Zhang and colleague [8] used the *virtual experimental approach* to investigate the effect of micro parameters, such as interphase strength and residual thermal stress, on fibre-reinforced composites (FRC) macroscale behaviour. Their version of the virtual testing scheme consisted of a four-step process namely: (a) generation of real microstructure of the test composite (b) computation

of composite constituent properties (c) progressive damage analysis (in explicit FEM) and finally (d) validation of predictions with experimental data. The above implementation agrees completely with the principles of micromechanical computational material science underpinning a virtual testing method.

Llorca and co-workers [18] reviewed the current state of knowledge of composite materials. This work presented a bottom-up multiscale modelling approach for undertaking high fidelity virtual tests of composite materials. To date, this version of the virtual testing represents, in our opinion, the most extensive, robust and holistic computational modelling framework for analysis of UD composites. The proposed strategy begins with in situ micromechanical and nanomechanical characterization of matrix and fibre-matrix interface mechanical properties to develop a detailed understanding of their individual nonlinear constitutive behaviour: this is achieved by performing nano-indentation matrix and fibre push-in/out tests to determine in situ matrix and fire-matrix interface mechanical properties respectively, whilst micromechanical tests are performed on the fibres to determine its mechanical properties. These nanoscale in situ characterizations – both dependent on the consolidation process - fall under *nanomechanics*. Such characterization is essential for each family of matrix and interface since the processing histories that UD composites are subjected to during the manufacturing stage cause the properties (matrix and interface) to vary markedly. The fibre properties were supplied by manufacturers and have been extensively characterized during the material/process optimization scheme of the organization. The findings at this microscale are systematically transferred to the mesoscale to inform ply- or lamina-level mechanics of UD composites. Finally, macroscale response is predicted using lamina-level simulation outputs. Such approach involves robust computation across different length scales. The three-step implementation requires three computational frameworks namely: *computational micromechanics, computational mesomechanics* and *computational mechanics.*

The challenge in the Llorca *et al* [18] variant of the virtual testing method is the onerous task of validating the simulation outputs at each length scale before such results are accepted at the higher length scale. The authors applied their virtual testing method to testing of unidirectional fibre reinforced polymers (FRPs) as well as braided composites. Extensive validation data were gathered from nano-indentation tests for matrix properties and fibre push-in tests for fibre-matrix interface properties. At the ply-level, the authors used a 3D RVE to assess the effect of reinforcement volume fraction, spatial distribution and shape on deformation and damage mechanisms of a typical metal matrix composite [38]. The authors also determined the failure locus of FRP plies reinforced with carbon or glass fibres [39-42] using a 3D RVE. Since the implementation was based on computational micromechanics, it was possible to extrapolate predictions outside the bounds of the experimental data i.e. assess effects of volume fraction, arrangement and shape of reinforcements on predicted

failure locus. This was impossible using traditional experimental approaches [28, 43, 44]. Comparisons of numerically determined failure locus with experimental data showed good agreement. Fracture resistance of a composite ply was also determined using the virtual test laboratory by explicitly modelling the interaction of crack propagation with microstructure of the FRPs and braided plies [45-47].

For macroscale predictions, the authors suggested using computational mesomechanics data as input to a homogenized macroscale laminate. Stiffness and strength (i.e. failure loci) values were derived from the mesoscale predictions. The numerically generated failure locus was applied to the laminate to determine the onset of failure and finally continuum damage mechanics used to predict damage evolution. Finally, the authors speculated on the benefits of a virtual processing route to be used in parallel with the above virtual mechanical testing route, as shown in **Figure 2**. The virtual processing route has also a multi-step implementation procedure comprising: molecular dynamics, kinetic theory micro-fluid dynamics, curing kinetics, etc at different length and time scales. Also, this route of analysis should incorporate the rheological properties of the polymer in its influence on the manufacture of the test composite. According to Llorca *e al*, this dual virtual testing and processing approach, should establish the roadmap of virtual testing in composite materials.

Mikulik *et al* [4] developed a virtual testing implementation, incorporating a virtual crack closure technique, for prediction of failure initiation locations and failure loads of UD composite materials containing multi-level delamination. Similarly, Irisarri, *et al* [48] used the FEM method to generate 'virtual test data' for strength of mechanically fastened CFRP composite joints. Traditional methods for strength prediction are based on semi-empirical models and a large test database.

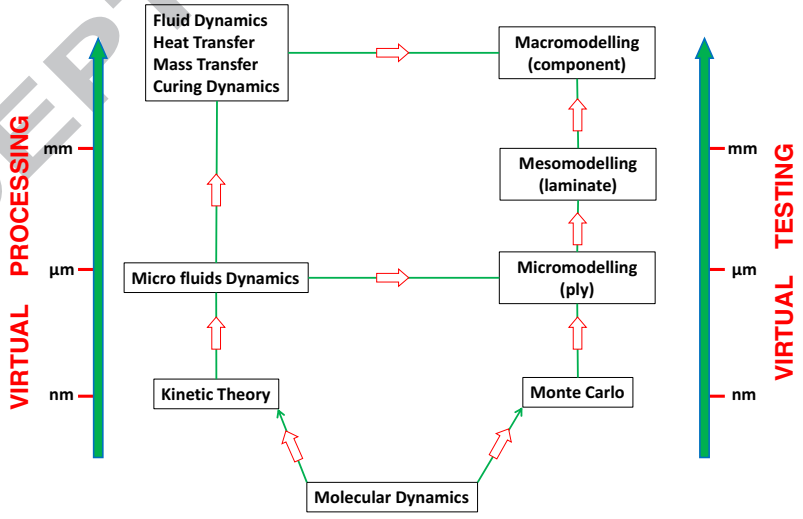


Figure 2: A multiscale simulation strategy for laminated composites comprising virtual testing and processing routes [18].

The use of virtual testing here has led to: (a) prediction of properties outside the bounds of the experiments, (b) the parametric studies on constitutive response of the materials and (c) material testing without expensive material redesign and testing strategy used in classical laboratory tests (trial and error strategy).

Okereke and Akpoyomare [11] developed another variant of the virtual testing scheme for prediction of a holistic set of effective elastic properties for UD composites. The authors used a computational micromechanics approach in their analysis. 3D RVEs with pseudo-randomly distributed E-glass fibre within a polypropylene matrix was generated using a MATLAB™ [49] algorithm developed by the authors called *Monte Carlo representative volume element generator* (*MCRVEGen*). The matrix and fibre constituents were modelled as isotropic linear elastic materials – assuming perfect bonding between the fibre and the matrix constituents. Periodic boundary conditions, originally proposed by Kouznetsova *et al* [50] for 2D RVEs, was extended for 3D RVEs. The authors used a combination of Python™ and MATLAB™ scripts to automate the processes involved from geometric models creation, boundary conditions application with respect to load cases and eventual bridging of the macro- and micro-fields predictions using a robust computational homogenization technique. The authors used the virtual test to predict all possible elastic properties of the UD composite investigated. The work also presented parametric studies on various aspects of the virtual framework. The authors concluded that the proposed virtual test scheme was a robust framework for investigating every aspects of the constitutive behaviour of UD composites, within an elastic loading regime, and most importantly was suitable for advanced virtual testing of this class of composites beyond the elastic regime, with the incorporation of robust constitutive material models.

4.1.2 Textile Composites

Virtual testing of textile composites has attracted significant attention in the last decade. Broadly, virtual testing in textile composites is divided into two strata: geometric modelling and numerical analysis methods. The former focuses exclusively on the architecture of the textile reinforcements without considerations to the mechanical behaviour and static boundary conditions (resulting from for example blank holders) of the reinforcement[51]. Geometric models can also be classified into those that are generated purely from the topology of the textile composites and those that are derived purely from the actual fibre architecture/geometry (often from x-ray computer tomography) [52]. The complexity of modelling the geometry of textile composites demands that accurate representation of their microstructure is essential if their mechanical performance is to be modelled effectively [53]. It is therefore not surprising that a large percentage of current works involving textile composites has focussed exclusively on model generation strategies. This review will consider both geometric and numerical approaches. The key publications chosen for review of virtual testing of textile composites were published in the last eight years.

One of the earliest models for describing the internal geometry of 2D- and 3D-woven textile composites called the CETKA-model was developed by S. V. Lomov [54-59]. The model was based on a minimum number of topological data like weave style, inter-yarn distance as well as yarn mechanical properties. The CETKA-model incorporated the principles of the Mori-Tanaka method for obtaining the homogenized elastic properties of textile composites [60] as well as the multi-level decomposition models of Vandeurzen [61]. Following the success of the CETKA-model, Lomov and co-workers developed robust software for geometric modelling of textile composites called *WiseTex* [59]. This advanced virtual testing tool integrated micro-mechanical response with permeability and structural analysis of textile composites spanning the micro-, meso- and macro-scale lengthscales. The *WiseTex* family of models established a unified description of geometry of unit cells and their translation to FE models.

Lomov and co-workers [62] developed a virtual testing scheme for textile composites based on meso-scale finite element modelling. This implementation built on previous successes by the authors in developing the *WiseTex* family of models. However, the current work was based on realistic reinforcement geometry representation and stress-strain state at the meso-level. Key elements of this implementation included: (a) meshing of realistic representation of internal geometry of reinforcements with actual volumes; (b) micro-homogenisation implementation of impregnated yarns; and finally (c) incorporation of realistic boundary conditions with periodicity of reinforcements adequately modelled. Following finite element analysis of the unit cell models, the resulting stress-strain fields become representative of the mechanical behaviour of the textile composite. This modelling strategy led to further analysis of damage initiation and evolution in textile composites. The authors believed that in order to establish a road-map for virtual testing of textile composites, it is expedient that researchers deal with the following issues: development of robust software for internal structure of reinforcements (as *WiseTex*); pre- and post-processing using FE models; implementation of representative (periodic) boundary conditions; multi-level homogenization techniques and development of damage initiation and evolution mechanics.

As a result of the complex architecture of textile composites, the associated shear deformation is often quite large, especially when subjected to combined load cases comprising shear and tensile/compression loading. Badel and co-workers [51] characterized this in-plane shear response using a finite element method for dry textile composites. According to the authors, tensile deformation in carbon fabric is about 1% while shear deformation can be as large as 0.872 rad. In order to develop a virtual model for determining large in-plane shear in textile composites, the authors emphasized the importance of choosing representative boundary conditions and appropriate mechanics of the yarn systems. In achieving the former objective, the authors used a periodic boundary condition (shown in **Figure 3**), similar to that proposed for 2D RVEs by Kouznetsova *et. al*

[50]; the model also incorporated inter-yarn rotation as shown in **Figure 4**. The combination of all these modelling features led to a numerically determined shear profile which is consistent with experiments. The authors identified a limitation to their study as being a problem of periodicity of material, such that at finite shear strains, a part of the deformed geometry leaves the deformed unit cell. Such a virtual test will lead to results which can inform the fabric-design stage of the manufacture of textile composites.

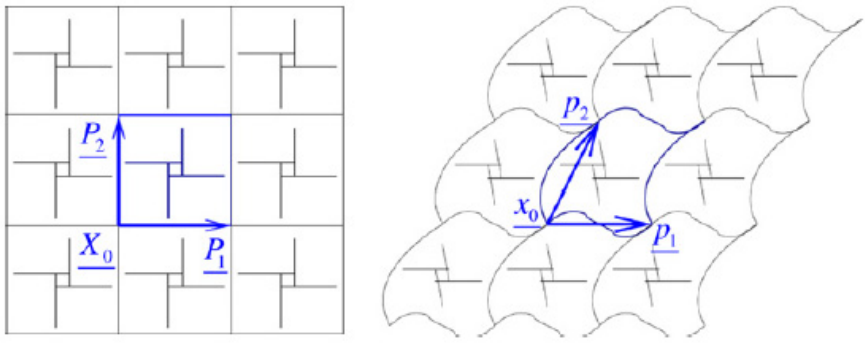
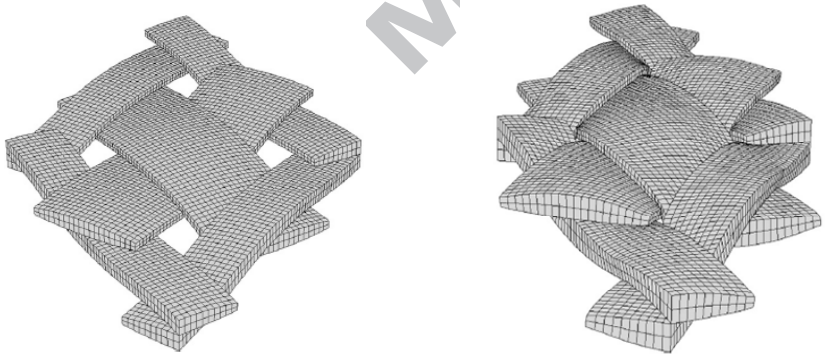


Figure 3: The representation of a periodic boundary condition for textile composites [51].



(a) (b)

Figure 4: Deformed geometries of two types of Representative Unit Cells (RUCs) of dry textile composites showing shear angles (a) $\alpha = 28^0$ and (b) $\alpha = 54^0$. Reproduced from [51].

Following the modelling philosophy of Badel, in 2010 Ernst and co-workers [63] developed a virtual test setup based on a multiscale analysis which uses the mechanical properties of constituents, glass fibres, and epoxy resin. In particular, the authors obtained predictions of strength of textile composites by incorporating an advanced constitutive matrix material model, a failure criterion and a strain softening algorithm: an improvement on Lomov's model [62] which neglected material

nonlinearity in all loading state but damage initiation regimes. The Ernst virtual model [70] consisted of representative unit cells tested within an FE scheme at both micro and meso-scales. At the meso-scale, yarns were modelled as fibre bundles which could be regarded as UD-composites. The virtual test models were validated against existing experimental data and were found to give reliable predictions as shown for a three-point bending test in **Figure 5**. Inter-fibre failure (IFF) and fibre failure (FF) as well as onset of degradation in transverse directions were predicted accurately using the virtual tests. The authors concluded that such multiscale virtual tests should be able to complement and replace experimental tests; this is chiefly because of their robust predictions and wider design, characterization and testing possibilities.

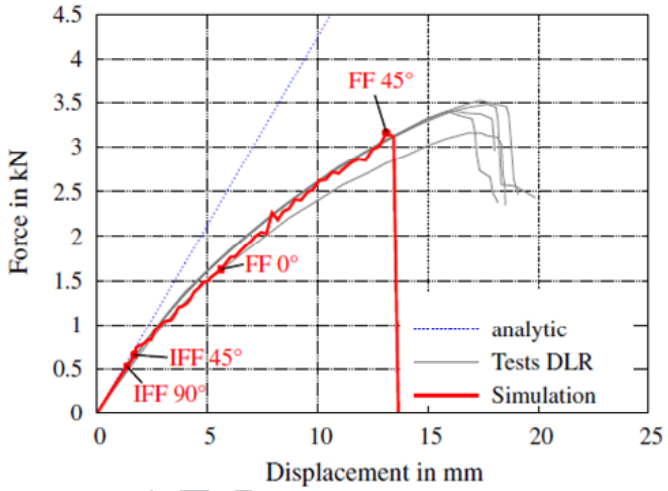


Figure 5: Comparison of analytical, experimental and virtual tests (Ernst et al) predictions of a typical three-point bending test. Reproduced from [63].

Rolfes [64] subsequently improved the prediction of multiscale progressive failure of textile composites by Ernst and co-workers [63]. The authors developed an orthotropic layer-based failure criterion for modelling the progressive failure of non-crimp fabrics. Virtual material tests (based on meso-mechanical unit cells) were used to determine strength and stiffness parameters needed for the failure criterion. The authors were therefore able to assess the effect of lower scale inhomogeneities on macroscale material behaviour, using a multiscale modelling philosophy starting from knowledge of properties of the constitutive response of the constituents. According to the authors, the major improvement in their work was the ply-wise analysis of single textile layers by virtual tests which is challenging and difficult to determine from laboratory experiments.

Smilauer *et al* [47] extended the multi-scale analysis for virtual testing of textile composites by incorporating fracture prediction in the mechanics of braided composites. The study investigated

the prediction of fracture energy, G_f and effective length of the fracture zone, c_f, of two-dimensional triaxially braided composites. **Figure 6** shows the multi-scale nature of the approach proposed by the authors. The authors queried the easy choice of 'bottom-up' models where a subscale simulation yields input data that is passed in form of a constitutive law or homogenized property into a macroscale continuum point (e.g. an integration point of an FE scheme) [47]. Such hierarchical models are well posed for solution of elastic and plastic hardening behaviour of heterogeneous materials however they are not suitable for prediction of softening fracture behaviour. This is because of the problem of localization of softening damage with their associated characteristic length and size effects [65, 66]. This problem lies in the difficulty (unresolved still) of correctly identifying material characteristic lengths from mesoscale simulations before transmitting same to the macroscale predictions especially for problems involving material degradation as fracture or softening damage [67].

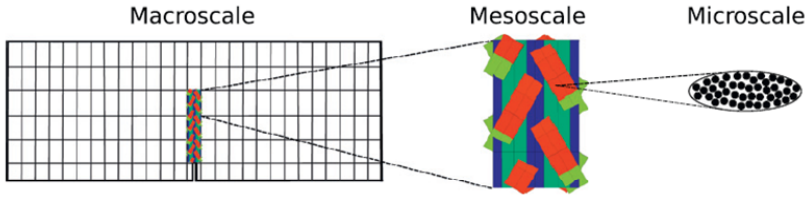


Figure 6: Illustration of the three-length scale representation adopted by Smilauer *et. al.* Reproduced from [47].

An alternative to the 'bottom-up' models is the 'concurrent' model [33, 68] which identify regions of potential softening and replace these with unit cells at the subscale incorporating the correct fracture mechanisms. The Smilauer and co-workers [47] 'concurrent' model composed of axial fibre tows, bias (or braider) fibre tows inclined at angle, ϕ pure matrix tows and connecting truss (or bar) elements [47]. The authors used truss (beam) elements to model the matrix parts of the model. The trusses are essentially linear connections between specific nodes on axial tows to contacting nodes on bias tows. The truss elements are assumed to behave as an elastic-damage spring. The authors specifically treated the matrix parts as a continuum without any sub-divisions unlike the axial and bias tows. This implementation, in the opinion of the authors, was a computational choice which removed the necessity of identifying the correct material characteristic length for the softening damage of the matrix. Although this approach is a bit odd, the authors showed their predictions to fit experimental data well. It can only be seen as another phenomenological approach for identifying or not a localization limiter for simulations involving material degradation/softening damage. Until better approaches for correctly identifying material characteristic lengths from mesoscale simulations are available, every author's approach will represent an attempt which will be acceptable pending the discovery of better approaches. Also, the Smilauer and co-workers' approach is limited by the

requirement for *a priori* knowledge of the crack path. Here, representative unit cells (RUCs) at mesoscale were placed in the propagation path of the crack as a replacement of the former macroscale elements, thus leading to prediction of fracture energy, G_f and effective process zone size, c_f.

At the microscale, only inhomogeneities below 5 microns were modelled. Rule of mixtures was used to predict elastic properties of axial and bias (or braider) tows based exclusively on properties of the fibre and matrix constituents. The RUCs were modelled at the mesoscale comprising of axial fibre tows, bias (or braider) fibre tows inclined at a defined angle, ϕ ; pure matrix tows and connecting truss elements [47]. At the macroscale, predictions from simulations of a notched three-point bending test were compared with corresponding experimental data. The modified 'concurrent' modelling philosophy adopted by the authors identified the crack path substituted a collection of RUCs with this path. Several simulations were carried out for different numbers of RUC collections. Parametric studies of boundary condition effects of predicted elastic properties were carried out. Similarly, simulation results from virtual fracture tests of the notched beams yielded several conclusions : (a) fracture initiates in matrix region on load application (b) shear damage occurs in the bias tows at 50% peak load; (c) bias tows may fail in tension close to peak loads, as illustrated in **Figure 7**.

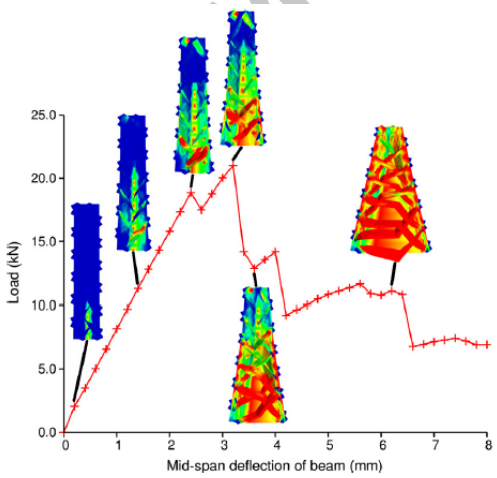


Figure 7: Results of simulations of notched three-point bending test incorporating three embedded RUCs and bias tows of angle 30^0. The contour plots show magnitude of damage within the composites. (Please refer to web version of article for coloured version of the figures). Reproduced from [47].

As a result of the relative success of their unidirectional composites' multiscale virtual testing approach, Llorca and co-workers [36] also developed a virtual testing scheme for braided textile composites. Typical results from their virtual test of some textile composites are shown in **Figure 8**.

The modelling philosophy used here is consistent with the approaches of Badel *et al* [51] and Smilauer *et al* [47] discussed previously where an RUC of the textile preform is used in simulating the mechanical behaviour of the fabric using appropriate boundary conditions. The authors agree, as already stated, with the requirement for using RUCs derived from robust geometric modelling of the architecture in the determination of elastic properties for 2D and 3D textile composites. However, beyond the elastic regime, the determination of failure locus of the textile composite becomes more complicated because of the diverse nature of the damage mechanisms in textile composites.

Damage in textile composites is a cumulative effect of many underlining mechanisms some of which include (a) inter- and intra-yarn bundle cracking (b) kink-band formation on fibres within vicinity of bundles crossings; (c) fibre pull-outs; (d) onset of delamination; (e) arresting of delamination when delamination cracks meet yarn bundles of different orientation and (d) micro-cracks in matrix pockets between yarns [18]. Macroscale damage is therefore observed as a coalescence of these diverse micro and mesoscale failure mechanisms; herein lays the complexity of damage modelling of textile composites using a multiscale analysis. Llorca proposed the use of cohesive zone elements for such interface-related failure mechanism at the mesoscale. However, the matrix-originating failure mechanisms were incorporated at the fibre-matrix microscale level through a constitutive equation. Based on the modelling approach described above, predicted macroscale responses using virtual 'fracture' tests on notched three-point bending geometric models were consistent with experimental data.

Another virtual testing scheme for textile composites developed in 2012, with a emphasis on geometric modelling, was developed by Stig and Hallström [10, 69]. The virtual testing framework developed by the authors was designed to determine the elastic response of three-dimensionally (3D) reinforced woven composites. [10, 70]. Homogenized elastic properties of the textile composites were derived using the virtual framework. The study was limited to representative unit cells (RUCs) with four instances of warp, weft and binder yarns. The authors did not give any objective justification for this choice. It is therefore debatable if the predicted elastic response is independent of RUC size.

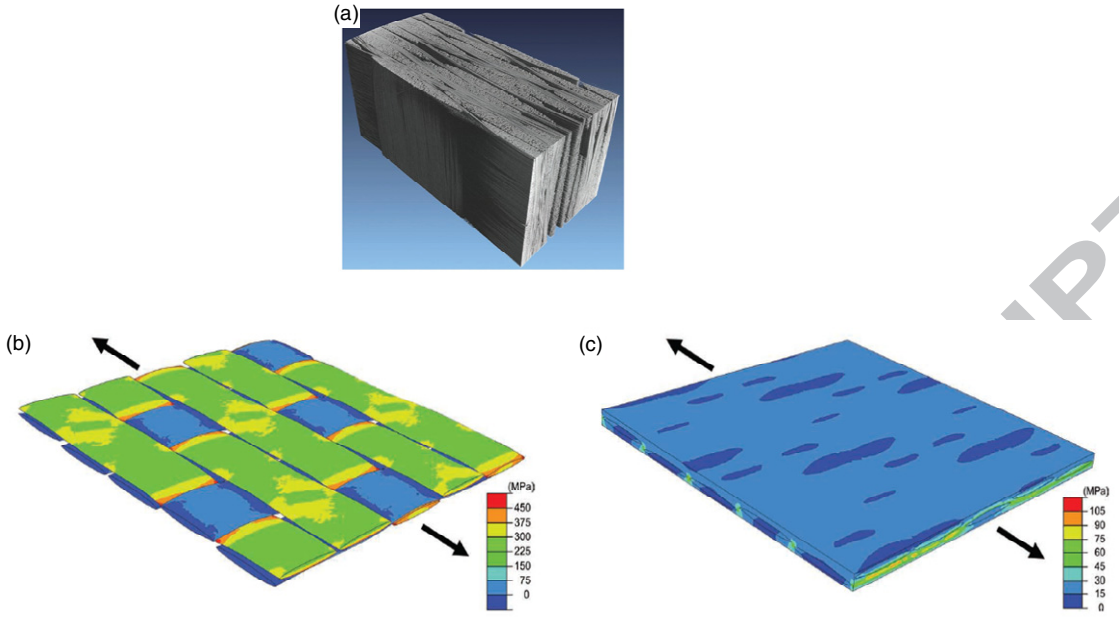


Figure 8: Virtual testing of textile composites showing: (a) X-ray microtomography – without matrix illustrating architecture of yarns; (b) contour plots of stresses in fibre yarns only of a typical RUCs of five-harness satin fabric composites undergoing tensile deformation and (c) contour plots showing stresses in matrix region only for same textile composite. Reproduced from [36].

The main distinction of the Stig-Hallström approach over other geometry-generating approaches is that it is designed for textile composites where the weave architecture is truly three-dimensional. For such cases, yarn cross-sections change shape, size and orientation within the complex internal geometry of the textile composites. Volumetric overlaps of bundles arise if the variations in yarn shapes, trajectories, etc are not adequately modelled. Unfortunately, the *WiseTex* models, and some of the previous virtual testing schemes will not be adequate for dealing with such 3D woven composites since there is the underlining assumption of the yarn bundles having constant cross-section. The Stig-Hallström virtual testing framework generates geometric models (see **Figure 9**) numerically without undue reliance on matrix-infiltrated physical weave structures determined using computer tomography. Rather, an automated geometry-generating algorithm was developed which takes input from initial circular cross-sectional profiles determined from the *TexGen* software [71, 72].

Yarns within the *TexGen*-generated geometric model follow trajectories, defined by splines, which are subsequently modelled as strongly anisotropic inflatable tubes: representative of the yarn bundle. Periodic meshes of the RVE surfaces were derived for the periodically repetitive RVE geometry of the 3D woven model. Predictions of effective elastic proprieties using the generated geometric models produced a 10% discrepancy when compared with experimental data. This was attributed to the RVE-based analysis being regular unlike real materials which contain appreciable irregularities due to the

manufacturing process. This version of the virtual testing framework could be extended to investigate onset and evolution of damage in 3D woven composites. Simulations of mechanical responses of the RVE gave predictions of Young's modulus which agreed with experiment although there was a 10% discrepancy. This was attributed to the RVE-based analysis being regular unlike real materials which are not always regular due to the manufacturing process. This version of the virtual testing framework could be extended to investigate onset and evolution of damage in 3D woven composites.

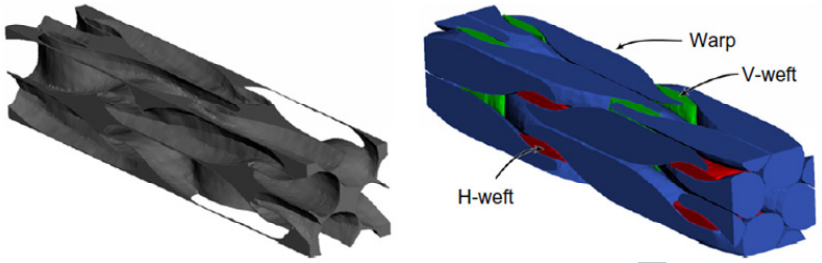


Figure 9: Stig-Hallstrom RVE representation of a 3D woven composites showing (a) pure matrix only (b) yarn bundles with warps and two directions of wefts. Reproduced from [10].

The discrepancy posed by the Stig-Hallstrom approach was overcome by a *virtual specimen* algorithmic generator developed in 2012 by Rinaldi and co-workers [52]. This work focussed exclusively on geometric model generation for subsequent use in thermo-mechanical performance and damage evolution analyses. The complex topology of physical textile composites introduces stochastic variations which are generally not captured in many numerical representations of the microstructure of textile composites. The central philosophy to the Rinaldi and co-workers' approach is that the statistics of the microstructure are close to those obtained experimentally, often from x-ray micro-tomography [73-75], hence they are principal parameters in developing any geometric model.

During the geometric model generation, a Monte Carlo style algorithm based on Markov Chain operators for generating replicas of textile composites was used [74]. The principle was originally developed for 1D tow loci of the textile composites. However, Rinaldi and co-workers have augmented the principle by creating trial 3D tow representations which were subsequently converted to *physically valid virtual specimens* [52]. Interpenetrations between tows generated by this means are common and the authors developed a set of topological rules for automatically removing such interpenetrations. Statistical variance of the tows was achieved using the Monte Carlo method. The analysis was based on a meso-scale with the fibre tows modelled as homogeneous systems. The authors acknowledged that a more accurate approach will require a mesomechanical analysis of the tows incorporating a different probabilistic formulation for capturing the statistical variance of the tows. The authors demonstrated the suitability of their method towards virtual testing of textile composites using a 3D angle interlock composite with carbon fibre tows in a ceramic matrix. A

typical virtual specimen derived by the Rinaldi and co-workers approach is shown in **Figure 10**. A drawback of this approach is the initial prohibitive cost of obtaining actual representations of the microstructure using, as in this case, synchrotron x-ray micro- computed-tomography.

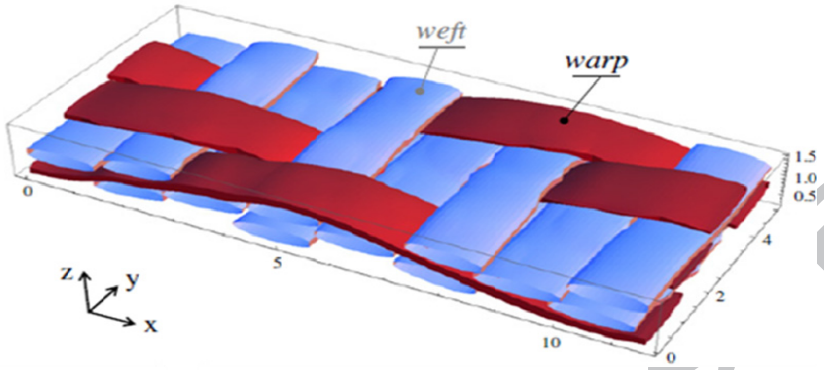


Figure 10: A typical virtual specimen of a 3D angle interlock ceramic matrix composite following removal of tow interpenetrations. Reproduced from [52].

4.1.3 Cement, Concrete, and Ceramic Composites

The FRPs and textile composites previously considered account for the bulk of industrially relevant composites and form the bedrock for virtual testing of composite materials. This section is dedicated to other types of composites which can include: cements, concretes, and ceramic composites. They have been grouped together under a single class of heterogeneous materials because of the similarity of their microstructure which generally comprise of irregularly shaped inclusions within a matrix medium. Fibrous ceramic composites and metal matrix composites (MMCs) with ceramic reinforcements will also be included in this section. In all cases they show multi-phase, random, complex microstructure [76] while in most cases, exhibiting brittle failure and consequently similar predictive modelling approaches are used for these classes of composites. Studies dealing with the virtual testing of this class of material are few. This section presents some of the work in this area published in the last decade.

One of the earliest studies in this area was by Garboczi and co-workers [76] which focussed on cement and ceramic composites. A distinctive feature of concrete is that its properties continue to evolve with time and modelling should incorporate this time-dependent response. Virtual testing should aid the prediction of properties by including constitutive features of time-dependent evolution of initial mechanical, physical and chemical properties. The Virtual Cement and Concrete Testing Laboratory (VCCTL) (refer to **Figure 35**) is a typical virtual testbed dedicated to predicting the properties of cement and concrete based on inputs derived from experiments [15, 76]. The VCCTL-approach was not aimed at ending standardized experiments; because reliable virtual testing – in this

case – depends on well-characterized empirical data. Hence predictions from the VCCTL were complementary to physical experiments.

Key features of the VCCTL include the following:

a. *Material Characterization:* The Garboczi and co-workers' approach starts at the length scale of the cement and mineral admixture particles [76]. The main input here is the particle size distribution (PSD) obtained by laser diffraction. Since the hydration behaviour of cements originates at individual particle length scales, a clearly defined PSD is a crucial input parameter for the VCCTL hydration model [76]. Using SEM and x-ray microprobe analysis, the authors determined the realistic PSD for cement. Subsequently, the information was reconstructed into a virtual 3D domain (**Figure 11**) with a typical characteristic distribution of particles (for chemistry and shape) in a cement-paste microstructure before onset of hydration. As well as particles, it is also pertinent that a realistic representation of aggregates be made in order to determine accurate concrete properties. By a combination of x-ray computed tomography and mathematical analysis, developers of the VCCTL modelled fine and coarse limestone aggregates.

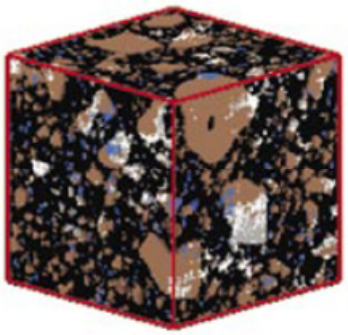


Figure 11: A virtual test specimen of concrete generated from VCCTL showing the multi-phase, random, microstructure of concrete. Reproduced from [76].

b. *Yield Stress and Plastic Flow of Concrete:* The VCCTL was also designed to determine the yield stress [77] and plastic viscosity of concrete. The challenge for virtual testing of concrete lies in the admixture of materials crossing different length scales from micrometre-sized cement grains up to coarse aggregates 20,000 times larger than the micrometre scales of grains [76]. The VCCTL uses a combined theoretical-experimental approach to undertake the virtual testing of concrete properties.

c. *Hydration Behaviour:* The VCCTL also incorporates a hydration model which is applied ~~on~~ to a representative 3D packing of cement particles (with characteristic particle shape and

chemical phase compositions). The model allows for dissolution of some of the cement particles which results in a hydrated 3D microstructural image of cement paste. Such a hydrated image is therefore used as input for determining property values such as: set point, heat generation, semi-adiabatic temperature rise, chemical shrinkage and self-desiccation and ionic diffusivity [76]. Finite element approaches can be used to determine elastic properties using the same hydrated 3D microstructural image of cement paste; as exemplified by results for dynamic moduli obtained from the VCCTL which agree well with experimental data. A similar approach will apply for computing the elastic moduli of concrete.

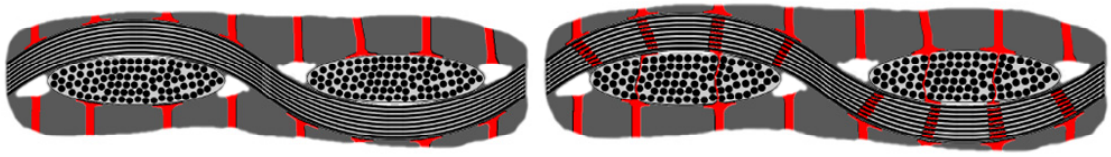
d. *Compressive Strength:* The VCCTL was used to determine compressive strength of cement based on a comprehensive model of the microstructure. The microstructure is enhanced using the hydrated 3D microstructural image of cement paste. In order to accurately predict compressive strength, multiscale strength of materials techniques were implemented at the microstructural lengthscale. The effect of moisture on the strength values was modelling using a hydration model based on the underlining Power's gel-space ratio theory [76]. The combination of representative microstructural information and a hydration model were able to determine compressive strength for any degree of hydration both for Portland cement and blended cement systems.

e. *Degradation mechanisms of cement:* The VCCTL software has been used to determine the degradation mechanism at microstructural level of cement by simulating the attack of sulphate or chloride on the cement paste's microstructure. There is a need to use similar virtual testing approaches to determine the durability of concrete. Developers of VCCTL are exploring this research area and considering linking VCCTL with SIMCO Technologies durability project (headed by Jacques Marchand in Université Laval, Canada). In this way, the durability of concrete could be predicted without reliance of, often time consuming, conventional tests.

According to the developers of the VCCTL, in order to obtain reliable predictions from a virtual testing scheme, high quality inputs derived from carefully designed experiments are essential.

Another class of heterogeneous materials under this category is the ceramic matrix composites (CMCs). Genet and co-workers [78, 79] developed what they described as a "virtual material" which is a multiscale multi-physics model for lifetime predictions of the constitutive response of CMCs.. The predictive tool was divided into two key mechanisms: chemical and mechanical. The CMCs investigated were built from woven yarns of SiC fibres impregnated with a multi-layered ceramic matrix, as shown in **Figure 12**. They are described as self-healing materials since their strength

increases through the saturation and interphase-inhibition of multi-crack growths that appear in the intra-yarn matrix.



(a) (b)

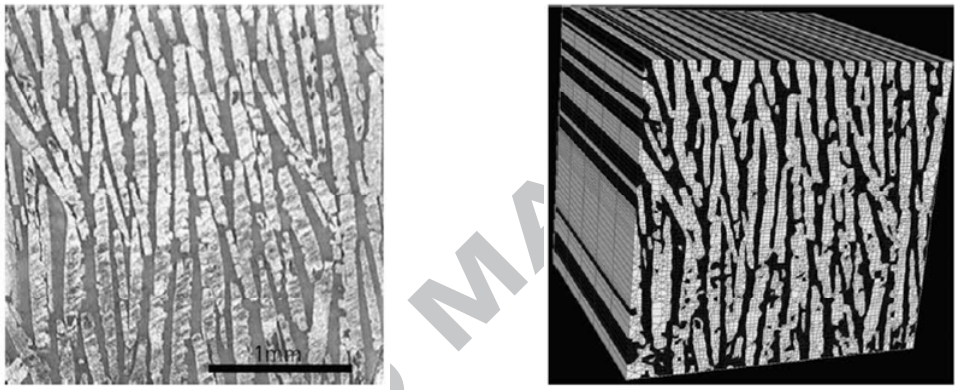
Figure 12: Illustration of a crack network within a self-healing ceramic matrix composite for (a) health and (b) cracked networks. Reproduced from [78].

The mechanical mechanisms of the virtual material are based on hybrid meso-cells at yarn-scale which is subsequently homogenized into a single framework. The underlining failure models were matrix-cracking (inter- and intra-yarn) and yarn-cracking. The chemical part of the model deals with sub-critical cracking of SiC fibres through stress-assisted oxidation [80]. As a result, even for stresses below the failure strength of the fibres, cracks are formed and propagated within the SiC fibres. A fracture mechanics based formulation [80, 81] was used to simulate these sub-critical crack propagations.

The virtual testing of CMCs, proposed by Genet and co-workers [78, 79], was focussed on isolated cracks and their effects on fracture performance of the test material. Lamon [82] continued the study by proffering a stochastic approach to study of effects of multiple cracks for a given CMC. The stochastic approach is based on the Weibull equation [83-85] for distribution of strengths for an entire volume of material experiencing multiple cracking. However, extra simplifying assumptions are included and these are (a) distribution of fragment strengths is required even for smaller and smaller flaws until saturation is achieved; (b) failure initiates at the weakest flaws and (c) the average failure strength of fragments is used [82]. This is what the author describes as *extreme value theory*. Explicit formulations for probability of fibre failure and matrix cracking in unidirectional CMCs were developed. Results showed good agreement with experimental data.

Metal-matrix ceramic composites (MMCs) are another class of composites that may appropriately be considered within this group of heterogeneous materials. Ziegler and colleagues [86] developed a multiscale homogenization method for determining the elastic properties of metal/ceramic composites with lamellar domain. They studied an MMC with statistically oriented domains of parallel ceramic platelets embedded inside a eutectic Al-Si-alloy [86]. The authors used a

multi-scale homogenization approach incorporating (a) finite element analysis at microscale (platelets-length scale) for geometric representation of the MMCs as shown in **Figure 13**; (b) meso-mechanical modelling of poly-domains of the MMCs. Young's moduli derived from the simulations were comparable with experimental data. The meso-mechanical modelling implementation (for poly-domains) can serve as a virtual testing framework for understanding the mechanical behaviour of MMCs. Similarly, Roy and colleagues [87] used micromechanical modelling supported by ultrasonic techniques to determine the elastic moduli of metal-matrix ceramic composites. The MMCs investigated here had complex interpenetrating microstructures and the elastic ~~moduli~~ properties determined (in all directions) included: Young's modulus, shear modulus and Poisson ratio.



(a) (b)

Figure 13: (a) Transverse micrograph of a metal-ceramic composites (b) 3D FEM mesh an MCC showing unidirectional arrangement of ceramic platelets. Reproduced from [86].

Pineau and co-workers [88] developed an advanced virtual testing approach for predicting the transverse multiple cracking of woven ceramic composites. The virtual testing investigated the localized response of individual tows within textile ceramic matrix composites (CMCs). The test material considered was a 2D SiC/SiC woven composite. The authors utilized 2D microscale models where individual tows, fibre reinforcements and their interphase regions were modelled explicitly, as shown in **Figure 14**a.

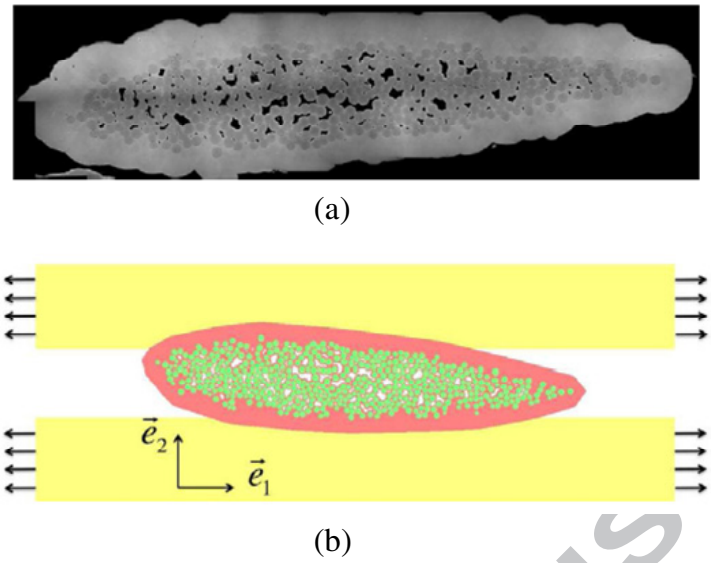


Figure 14: (a) Transverse micrograph of a single tow ceramic matrix composites used in generating virtual materials; (b) 2D loading arrangement for a meso-cell of the CMC. Reproduced from [88].

Damage in CMCs occurs in the following sequence: (a) inter-tow matrix cracking – depending on pore severity (b) cracking of matrix of transverse tows and finally (c) cracking of matrix of longitudinal tows. The load-bearing capacity of the CMCs is determined by the extent of matrix cracking of transverse tows, hence the virtual testing approach of the authors. Robust modelling of matrix cracking of transverse tows requires explicit modelling of two principal parameters namely: (a) the statistical distribution of failure data arising from heterogeneities (fibres, interfaces and voids) and (b) variability in constituent [88].

Pineau and co-workers derived an appropriate virtual domain for the FE model from micrographs of the test composite. Depending on the digital image analysis of the micrographs, different variants of the virtual material were derived (with varying contributions of fibres, voids, interphases and voids). Specific failure criteria were defined for capturing crack initiation of matrix and interphase. A virtual testing iterative process was used to detect the defects that contribute in a multiple cracking failure of the CMCs. Typical results using three distinct virtual materials are given in **Figure 15**. These numerical predictions agreed with corresponding experimental data for onset of matrix cracking in woven SiC/SiC composites. Additionally, the resultant crack patterns from the virtual tests were consistent with microscopy observations on the same material. Experimental data acquired from microscopy observations of matrix cracking indicated transverse tow matrix cracks initiate at a strain of about 0.08% [88, 89]. The virtual testing scheme has informed the possibility of testing individual tows, which is difficult to replicate in a physical experiment.

Finally, a most recent virtual testing scheme for CMCs was proposed by Tranquart and co-workers [90] for describing the microstructure and simulating the mechanical behaviour of complex CMCs. The structure is derived based on a pattern-based decomposition of the microstructure. Generalized Finite Element modelling (GFEM) multi-scale approach is used to simulate the mechanical response. All constituents of the CMCs are assumed to be brittle elastic and cracks formation and propagation is according to finite fracture mechanics.

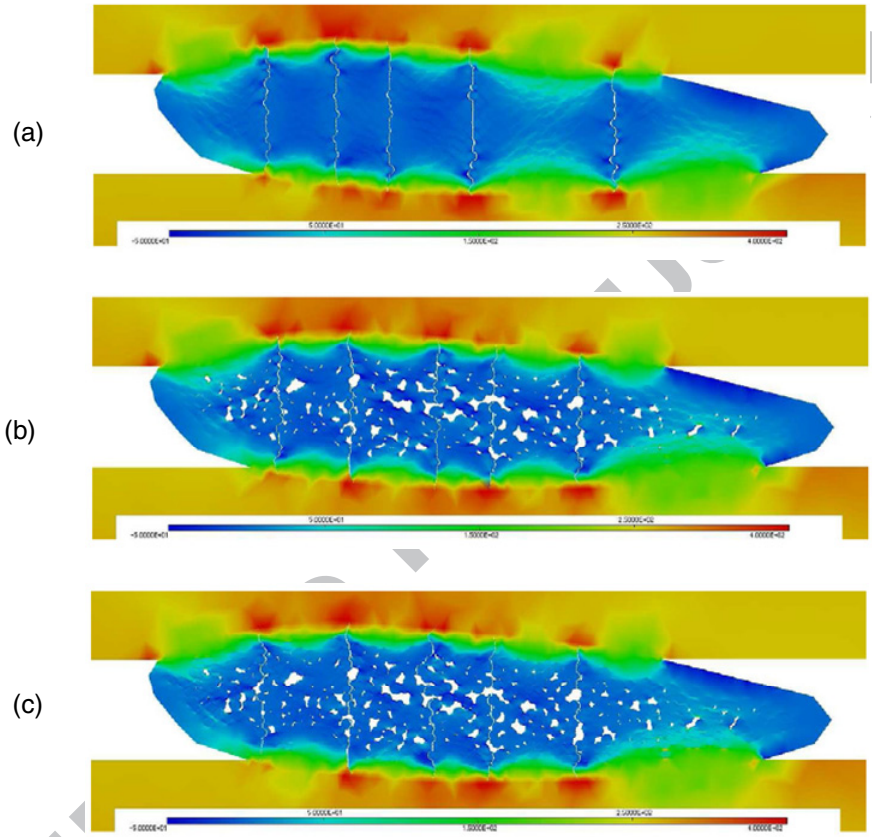


Figure 15: Multiple cracking patterns obtained by virtual testing of three classes of virtual materials where (a) fibres and matrix only (b) fibre, matrix and interphase and (c) fibre, matrix, interphase and voids. Reproduced from [88].

4.2 Cellular Materials

Another class of heterogeneous materials to be considered in this review are cellular materials which include sandwich core and foam structures. These materials are particularly attractive to the aerospace industries because of their lighter, cheaper and mechanically beneficial properties. However, current research into these materials involves a lot of trial and error testing of prototypes (with different geometric patterns of cells) to determine their mechanical properties. The range of cell geometries from honeycomb to various folded cores structures poses a testing challenge which is both

time- and cost-intensive [91]. Numerical approaches, involving finite element analyses, present an attractive solution to the preponderance of physical tests on prototypes. This also makes cellular materials attractive to the virtual testing approach where tests can be designed to give representative predictions of the relationship between cell geometries and mechanical properties. The following types of cellular materials are to be reviewed here: sandwich and foam structures

4.2.1 Sandwich structures

Sandwich structures consist of two thin and stiff layers with a central thick lightweight core. Over the last decade, Heimbs [91] has been pioneered research in virtual testing of sandwich core materials. Heimbs [91] provided a review of the emergence of virtual testing in sandwich core materials beginning with determination of elastic properties. Key studies in this area include work by Heimbs et al, Pan et al and Foo et al [92-94]. In recent times, improved computational power has led to virtual testing of cell wall folding mechanisms in the post-damage behaviour of test materials. Most existing virtual tests focussed on dynamic simulations using an explicit time integration scheme [91, 95, 96]. The cell walls were assumed to be regular in many of these previous works [97] however studies [98-100] have shown that cell shapes are irregular as a result of manufacturing processes.. Typical instances of numerically-derived irregular cell shapes are given in

Figure 16. Li and co-workers [99] carried out a virtual test for irregular cell shapes and non-uniform cell wall thicknesses. The study demonstrated that cell shapes and wall thicknesses significantly affect the stress wave propagation in the material, the strain-hardening, the plateau stress and the densification strain energy.

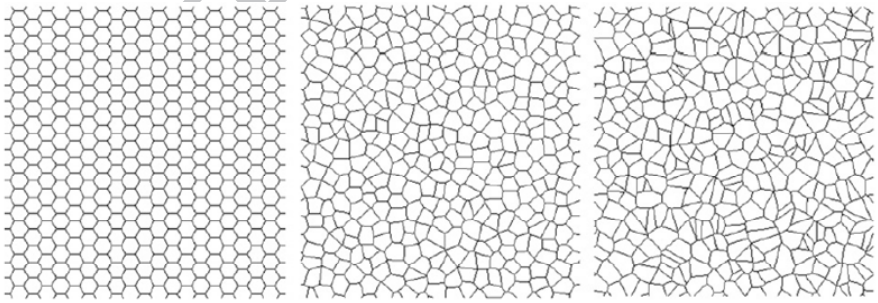


Figure 16: Numerically-derived instances of regular and irregular cell shape for a honeycomb [99].

All the previous virtual tests of sandwich cores materials were restricted in their predictive ability and modelling depth. Studies were limited to: a few core geometries (mainly hexagonal), aluminium cell walls, out-of-plane compression and elastic buckling of cell walls. Heimb's work [91] extended the virtual testing discussion of sandwich core materials to include many cell geometries (hexagonal and over-expanded honeycomb); folded cores -(made of Nomex®, Kevlar® and carbon

fibre composites); different material directions (in-plane, out-of-plane); different loading conditions (compression, tension, and shear), etc. The virtual test also addressed parametric studies relating to influence of model size, mesh size, loading rate, etc. to the mechanics of sandwich core structures. Finally, the author used virtual testing to optimize the design of a carbon folded core's geometry.

The virtual testing framework of Heimbs' includes: generation of geometry of sandwich core structure's finite element mesh (see examples in **Figure 17**); definition of cell wall material laws; implementation of imperfections, definition of boundary conditions and load cases. The geometric model was determined following a parameterized automated process. A cell wall material law was specified as a bilinear elastic-perfect plastic material for Nomex honeycomb cores. The author used MAT54 – an orthotropic elastic-perfect plastic composite material model in LS-DYNA – for the cell wall material modelling. Similar phenomenological approaches were taken to derive constitutive laws for the cell walls of the Kevlar and CFRP folded core materials.

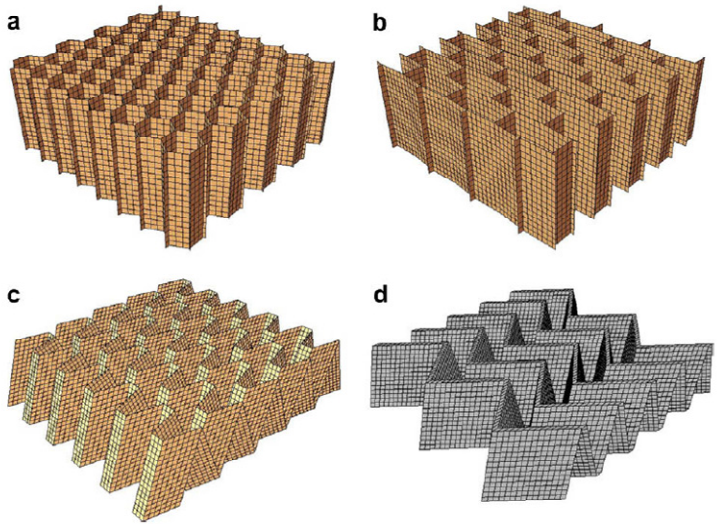


Figure 17: Numerically-derived 3D sandwich structures for: (a,b) Hexagonal and over-expanded honeycomb (c, d) Kevlar and CFRP folded cores. Reproduced from [91].

The cell imperfections seen in sandwich core materials were also incorporated into the virtual testing process by: (a) random distortion of the core's geometry prior to meshing and following meshing, (b) random distortion of cell wall thicknesses (by node-shaking) of finite element meshes and (c) variation of cell wall material properties for randomly chosen sets of elements. Boundary conditions and load cases were prescribed on the top and bottom thin rigid plates of the sandwich structure. Quasi-static simulations were carried out in LS-DYNA using carefully monitored mass-scaling such that the structural response was not altered by imposing a quasi-static loading regime for

a dynamic loading problem. Dynamic crushing load cases were also imposed on all four material types and a typical comparison of the experimental and virtual testing data on Kevlar folded core is given in **Figure 18**. Virtual test predictions agreed with experimental data, quantitatively and qualitatively, especially for compression across all materials.

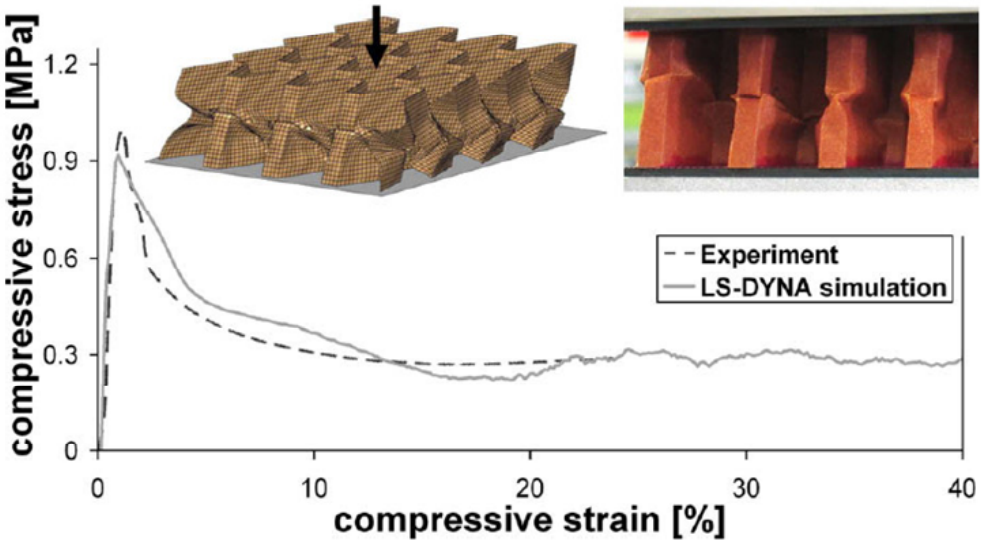


Figure 18: Comparison of experiment and virtual testing of Kevlar folded core structure based on compression loading condition. Reproduced from [91].

Giglio and co-workers [101] carried out similar virtual testing analysis as Heimbs but limited only to Nomex honeycomb core with hexagonal cell shape. Flatwise compression simulations were carried out and experimental results compared closely with predictions from these simulations. For a three-point load case, Giglio and co-workers [102] developed a virtual test for aluminium skins and Nomex honeycomb core. The aluminium skins were modelled using a Johnson Cook modelling framework [103] and a ductile fracture criterion [104]. The numerical load-displacement plots were analyzed further for key parameters: maximum force peak value, densification point, total absorbed energy up to densification, etc. Friction effects were also analyzed using the virtual framework and typical results from the study are given in **Figure 19**. The friction study showed that with increasing coefficient of friction, the failure mechanisms are different. These foregoing results and features demonstrate the suitability of a virtual testing scheme to replicate physical experiments and further inform micromechanical behaviour of cellular materials.

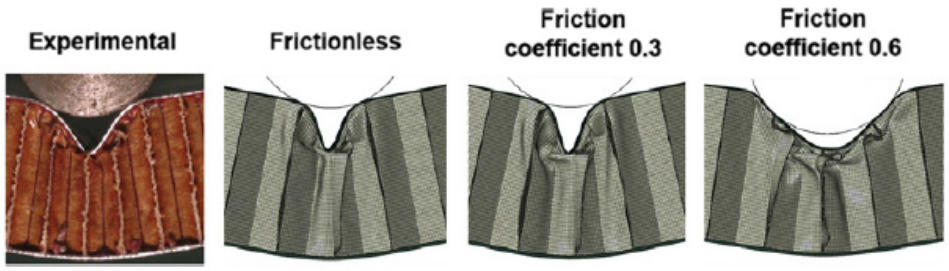


Figure 19: Comparison of experiment and virtual testing for three-point bending test for varying coefficients of friction on Nomex honeycomb core sandwich structure. Reproduced from [102].

4.2.2 Foam structures

Micro-cellular carbon foams are another class of cellular materials that have also been subjected to various forms of virtual testing. The micro-cellular carbon foams, also referred to as graphite carbon foams, are a new age material with mesophase highly ordered topological structures. They are known to exhibit superior mechanical and thermal properties and have become very attractive in several advanced applications (e.g. aircraft and spacecraft structures, low cost insulating and energy absorbing structures, heat insulation, lightweight packing materials, soundproofing, etc.). The foams are formed when mesophase pitch (coal, petroleum, or hydrocarbons) precursors are placed in a pressure vessel and subjected to a carbonization process of controlled temperature. Spherical (or often times elliptical) bubbles form to create the foam's topology which are subsequently heat-treated to form the final carbon-based foam structure [105]. Typical micrograph of the carbon foams is given in [106] showing the foam's microstructural components of size 10 μm.

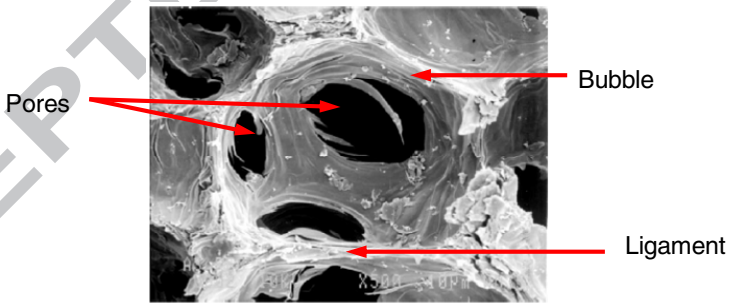


Figure 20: An SEM micrograph of a carbon foam showing the physical elements [106].

In recent times, the use of virtual testing techniques in understanding, altering and predicting the mechanical and thermal properties of carbon foams has become widespread. This is encouraged by the high costs of processing carbon foam structures as well as time required for physical tests. Digital models of carbon foams are expected to reduce the cost and times associated with physical tests [105]. Numerical representation of the foam's heterogeneous and anisotropic microstructure

presents a virtual testing challenge [107, 108]. The carbon foam geometry is often modelled by using CAD to create the bubbles and the foam structures as illustrated in **Figure 21** for a 4^3 mm^3 carbon foam model created in CATIA. Innovative algorithms have been proposed for determining the porosity of the carbon foams and correlated to micrograph data. James and co-workers [105] developed a typical virtual geometric model of graphite carbon foams based on 2D Monte Carlo style bubbles-representing intersecting circles algorithm. This was subsequently extended to 3D bubbles. Appropriate boundary conditions were imposed on meshed CAD models of the foam structure and subsequently, bulk properties of the foam material were determined. A typical compression simulation of an open-celled foam structure in ABAQUS is given in **Figure 22**.

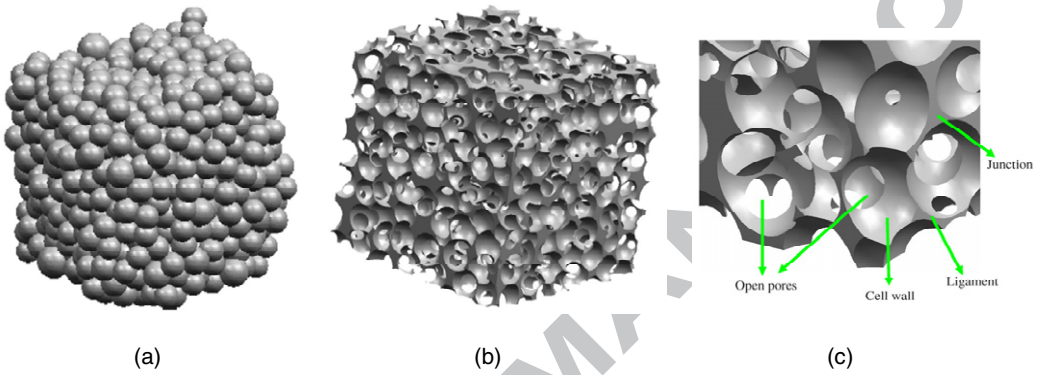


Figure 21: Virtual test material of a microcellular foam structure showing: (a) bubbles (b) foam structure (c) different parts of the foam structure [109].

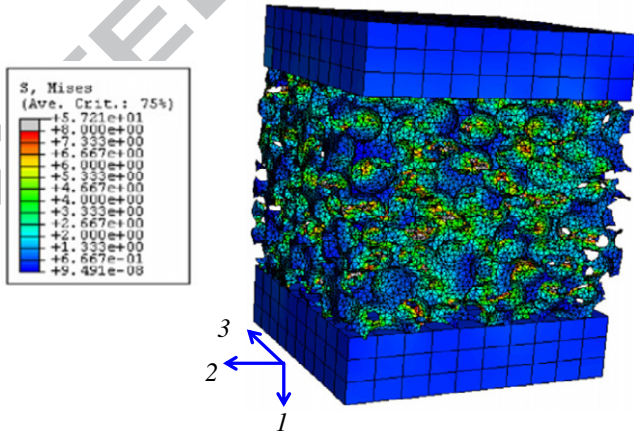


Figure 22: Contour plot von mises stress distribution from a compression test in ABAQUS of an open-celled foam structure [109].

Following the work of Sihn and co-workers [106] on the mechanical response of open-celled foam structures, the authors observed that the effective elastic properties of foam structures is dominated by bending mode associated with shear deformation [106]. The effective Poisson's ratios of the foams are independent of the Young's modulus of the ligaments but dependent on their

Poisson's ratio. The authors also developed a model generating algorithm similar to the James and co-workers [105] approach.

The comprehensive constitutive behaviour of foams can also be determined using a virtual testing scheme. The average, or "bulk" quasi-static compression of foams is divided into three regimes [110]. These three stages are : (a) at small strains - linear viscoelastic behaviour (b) at moderate/intermediate strains – plastic deformation, "yielding", and plateau region all at constant force with increasing deformation and (c) densification following dramatic stiffening of the material. The nature and extent of each of these stages varies from one foam type to another [111-115]. Features of first two stages have been modelled reliably by several authors however densification is particularly difficult to model due to the contact mechanics required at large deformation of foams.

Brydon and co-workers [108] used a virtual testing approach to model the complete densification of open-celled foam structures. They used x-ray tomography methods to determine accurately the geometry of the test specimen and subsequently used particle-in-cell (PIC) methods, requiring a particle representation of the foam microstructure (which sidesteps the contact mechanics problem). Typical compression simulations from the authors' study are given in **Figure 23**. The study investigated the effect of compression rates on the full foam model; hence the simulation results at both quasi-static and dynamic rates. The virtual test shows that bulk compression occurs before the compressing traction is registered on the boundary opposite the displacing plunger. Inertial effects following dynamic loading were found to influence the dynamic simulations such that higher tractions are observed under the displacing plunger compared with the quasi-static simulations. Physical experiments do not show this distinction as it is difficult to decouple the viscoelastic nature of the parent material from inertial effects of the foam microstructure [116-118]. The numerical predictions are consistent with experimental data with the exception of the dynamic loading studies. There is a need for further study on the mechanism of dynamic rate compressive behaviour of micro-cellular foam materials. Indeed, virtual testing as used in these studies provides a basis to explore the mechanics of foam behaviour across a wide range of strain rates – much more than experiments can provide.

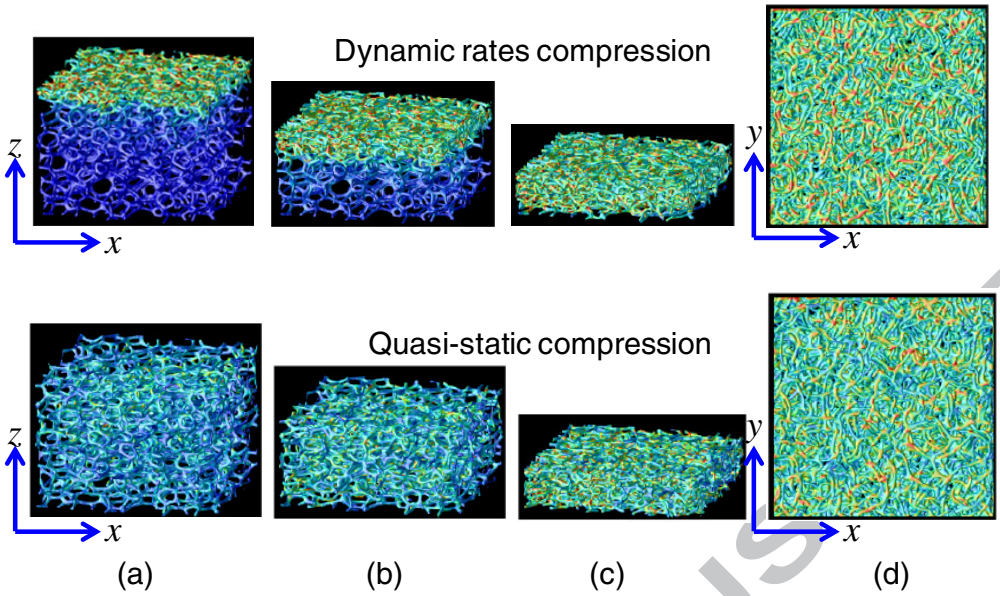


Figure 23: Virtual testing simulation of densification of open-celled foam structure showing material deformation at (a) 25% (b) 50% (c) 75% and (d) 90% engineering strain for imposed velocity at dynamic rates (*U=19.1* m/s) and quasi-static rates (*U = 1.91 m/s*). Note blue and red values shows small and large values respectively [108].

4.3 Biomaterials

In the context of this review, biomaterials are considered to be materials incorporating biological systems. The discussion will present the complex process involved in virtual testing of these materials – highlighting the geometry generating processes, meshing, boundary conditions and prediction of mechanical response. The literature considered here was published within the last decade. One of the most recent virtual testing framework for dealing with computational life sciences is by Neufeld and co-workers [119]. The virtual framework was designed for simulating and modelling complex biological systems in computational life sciences using inputs from medical images. The review of biomaterials will consider the following biomaterials: bone, skin, collagens, ligaments and wood.

4.3.1 Bone

Bone is a mineralized connective tissue which gives the body its structure and supports the body tissues [120]. In view of engineering mechanics, bone is considered a nanocomposites with a complex hierarchical structure, which culminates in the following excellent properties: high stiffness, strength and fracture toughness, coupled with low density [120]. Bone is made up of structures that span across nano-, micro-, meso- and macro-scales [121-123].

At nanoscale, mineralized collagen fibrils (MCFs) are formed from cross-linked collagen molecules, hydroxypatite (HA) nanocrystals, water and non-collagenous proteins (NCPs) [120, 124]. The overall behaviour of bone is strongly dependent on the MCFs as they form the structural building blocks of the bone. MCFs are the same for both cortical and trabecular bones. Single-layer lamella – made up of MCFs as well as ellipsoidal cavities called lacuna – make up a sub-microscale composition of bone. However, at the microscale, cortical and trabecular bones are composed of different lamellar structures: with mature cortical bones comprising osteons embedded in interstitial bone surrounded by circumferential bones while the trabecular bone consist of a porous network of trabeculae. At the mesoscale, the bone tissue is made up of dense cortical bone at its outer layer and a spongy trabecular (cancellous) bone in its interior [120]. The macroscale representation of bone is essentially the whole bone often from a few millimetres to centimetres.

Several modelling approaches have been developed for predicting the mechanical behaviour of bone [122, 123]. The approaches are dependent on the resolved/identified length scale of analysis necessary to execute the relevant investigation for the bone.. Seeman and Delmas [125] investigated the material and structural basis of bone strength and fragility at a nano-structural lengthscale. Other authors [126-128] determined elastic properties of bone by treating it as a nano-composite made up of lamellae comprised of MCFs with interconnections. The small sizes of collagen molecules and mineral platelets of bone present a difficult experimental characterization challenge at the nanoscale; therefore virtual testing techniques have evolved for this purpose. Typical examples are: Ji and Gao [126], Siegmund *et. al* [129], Ghanbari and Naghdabadi [130], Yuan *et al* [131], Luo *et. al* [132], etc. All these examples predicted elastic and damage behaviour of bone based on the mineral-collagen interaction on a nanoscale where the mineral is a matrix medium and the collagen is a reinforcement phase. Adequate boundary conditions and homogenization techniques were implemented to determine the constitutive response of bone based on virtual nanoscale RVEs. Predictions from the virtual framework were consistent with existing macroscale experimental data. Tate [133, 134] also developed virtual testing strategies for different multiscale responses of bone, ranging from mechanical deformation to flow in bones as well as molecular transport within bones. Virtual testing strategies have also been developed by Tate and co-workers for investigating the effect of bone porosity on effective mechanical behaviour of the bone.

Microstructural adaptation is a common feature of bones due to its response to increased or changing loads. The phenomenon of microstructural adaptation is also described as *bone modelling and remodelling*: it refers to processes by which bone adapts its shape and internal structure to external influences [135]. Virtual testing approaches (otherwise referred to as *in silico experiments*) have been utilized in investigating this biological process. Knowledge of the mechanism of bone modelling and remodelling is essential for combating bone diseases like *disuse osteoporosis* and *post-*

menopausal osteoporosis. The former condition is a form of bone losses driven by bone mechanics while the latter is a hormone-driven bone loss especially in middle-aged women. Both diseases require prolonged data acquisition which is critical for understanding the associated microstructural adaptation. Virtual testing offers a route towards understanding these microstructural mechanisms. In particular such *in silico* approaches have started relating the mechanical properties of bone to the underlying cellular processes – thus developing a field of study called *mechanobiology.*

Initial virtual tests for macroscale prediction of bone modelling and remodelling were based on continuum models where the microstructure was described essentially by its apparent density only. However, later models recognized the microstructure of cortical and an intricate trabecular structures; particularly their simultaneous evolution with age or loading conditions [136, 137]. Stochastic continuum approaches have also been added to predict the spatially diverse properties of bone. These continuum models have been implemented as both 2D and 3D finite element models [138, 139] for predicting age-related decrease of bone mass and strength. Most recently, Jang and Kim [137] developed a computational framework that simulated the simultaneous adaptation of cortical and trabecular bone types in human proximal femur with age. Results from the study are given in **Figure 24** which shows the strain energy distribution contour plots.

The microstructural adaptation in the Jang-Kim virtual framework was described by the authors as *design space optimization* (DSO) and *surface remodelling* which allowed for simultaneous movement of the periosteal and endosteal surfaces [137]. This numerical geometry – representative of a complete architecture of cortical and trabecular bone – was subjected to geometric changes following remodelling. Morphological changes in the bone microstructure following remodelling were quantified using strain energy density (SED). Prior to remodelling, the SED changed from a non-uniform distribution as shown in **Figure 24**a to a structurally efficient state depicted by the uniform SED distribution contour plot of **Figure 24**b. A further study of SED distribution for trabecular bone showed the initial configuration did not have a preferential axis of orientation but in both cortical and trabecular bones, the final SED distribution were aligned with the dominant loading directions. The proximal femur was also observed to be stronger and stiffer. As a result of age, bone adaptation led to bone being able to sustain higher loads. Likewise, this explains disease conditions such as osteoporosis where bone adaptation is inhibited leading to compromised bone integrity.

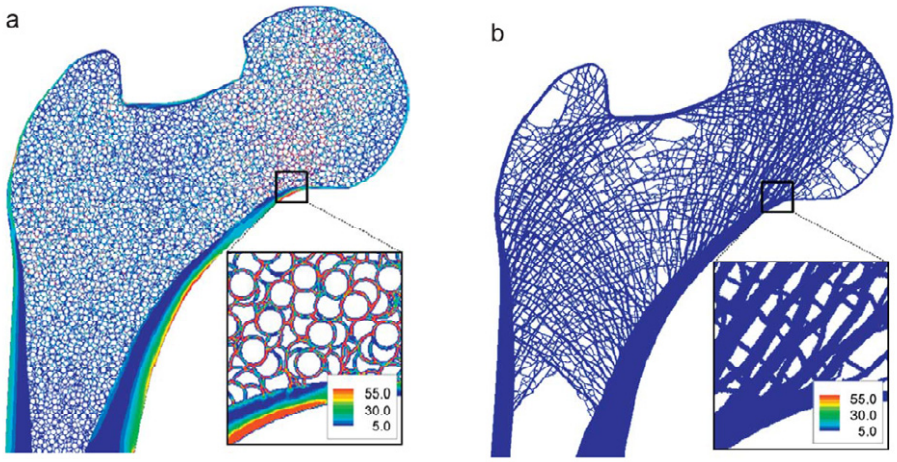


Figure 24: *In silico* simulation of age-related bone remodelling showing:(a) initial and (b) final strain energy distribution [137].

Christen *et al* [140] proposed a validation procedure for typical bone remodelling algorithms. The validation experiments are sets of well controlled experiments for determining the mechanical properties of fully and partially developed bone. Results from the *in silico* experiments and physical experiments were comparable for different bone micro-architectures subjected to a common loading history. However, the validation of *in silico* experiments using density-based approaches such as the Jang-Kim one has been questioned since such density-based validation lacks sufficient detail in accounting for the tissue loading inhomogeneity seen in bone microstructure [141-143].

Another class of virtual testing framework for predicting the mechanical response of bone is what has been described by the authors as *continuous computational multiscale model* [121, 144]. The essence of this virtual framework is to serve as a *computerized virtual biopsy system for bone diagnosis* by integrating 3D geometric modelling with multiscale finite element analysis of bone. The implementation mirrors the underlying hierarchical structure of bone ranging from a seemingly homogeneous macroscale (with low genus and low topological complexity) through a mesoscale or intermediate scale (comprising single or groups of trabecular or cortical bone) and then finally at microstructural scale (comprising of mineralized collagens, etc). This *continuous computational multiscale model* is illustrated in **Figure 25**. This approach enables continuous transition between the different scales by incorporating successive refinements of the mesoscale. Geometric representation at each scale is obtained using reconstructed μCT/μMRI images of bone. The geometric model of bone is developed based on a three-step process shown in **Figure 26**.

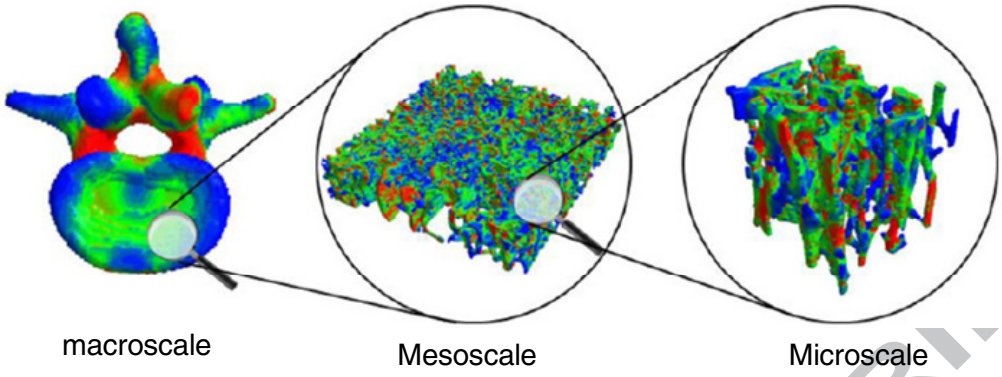


Figure 25: Illustration of scale differences required for a *continuous computational multiscale model* of bone [121].

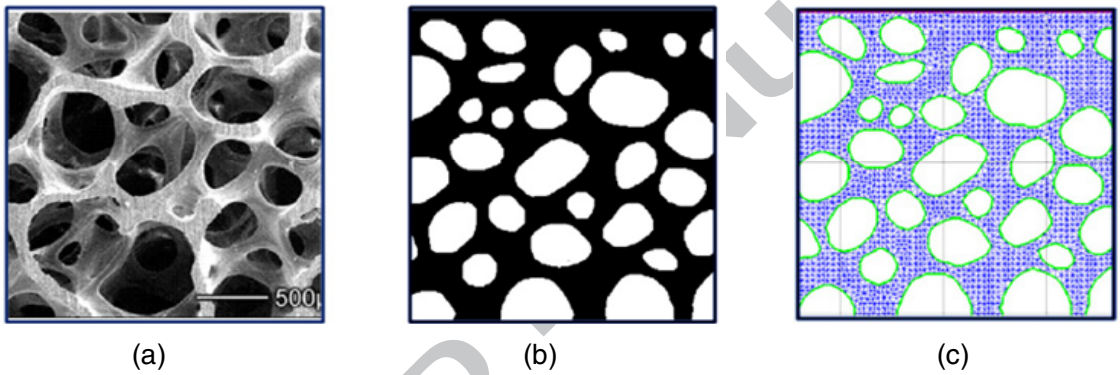


Figure 26: A three-stage numerical geometry generation for bone illustrating a 2D implementation: (a) μCT medical image (b) digitized image segmentation and (c) equivalent finite element mesh [121].

In order to relate the essentially isotropic macroscale material properties of bone to anisotropic material at the microscale, a correlation between porosity of geometrical models and their local material properties was defined [121]. This correlation was a fourth-order polynomial that relates the effective material properties with the porosity of the bone material at the given length scale: thus determining equivalent local material properties for geometric models at different levels of resolution. Homogenization techniques were used to derive effective elastic properties of the bone structure at the structural length scale. Other similar approaches [145] have treated the macroscale bone material as orthotropic and used FEA to determine effective elastic properties of bone.

Representative analysis of bone based on the Podshivalov and co-workers [121, 144] approach demands extending the above 2D virtual domain to a 3D space. The use of high resolution 3D models (from μCT reconstructions) would be ideal; however, high computational complexity and

large memory demands are limitations hindering such approaches. Instead, the authors used a domain decomposition approach [146] by dividing into sub-domains where an elasticity problem is solved in parallel. This sub-domain is described as the *model domain* and can include a single slice of a vertebra as shown in **Figure 27**a. The compilation of individual model domains into a single domain assuming non-overlapping domains creates a multi-domain representation of the entire bone/vertebra as shown in **Figure 27**b. Similarly, homogenized multi-domain material properties were derived and used for virtual testing of the bone. Results from this study were consistent with published experimental data. This multi-scale FE approach can be adapted for the modelling and analysis of materials characterized by irregular and stochastic microstructures [121].

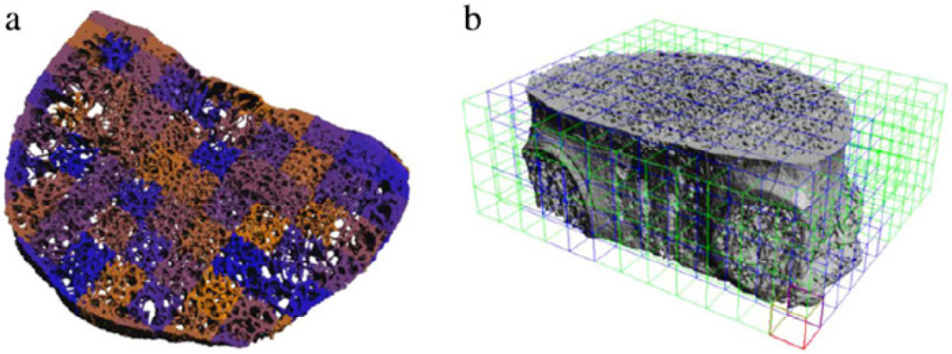


Figure 27: A domain-based multi-scale analysis of bone showing (a) single sub-domain slice representing a single model domain and (b) multi-domain of the entire vertebra [121].

4.3.2 Skin

Skin is a pseudo-solid composite microstructural material comprising two layers: the dermis and the epidermis [147] – both of which are inhomogeneous in terms of structure and composition [148]. According to Zöllner and co-workers, skin is a highly dynamic auto-regulated, living system that responds to stretch through a net gain in skin surface area [147]. The important mechanical properties of skin include: extensibility (stretching capacity), resistance to friction and response to lateral compressive loading [148]. These properties evolve continuously with species, age, exposure, hydration, obesity, disease, location and orientation of skin [149]. These mechanical properties show general anisotropy, nonlinearity, viscoelasticity, incompressibility and plasticity [148, 150].

The complex behaviour of skin as well as its heterogeneous composition poses a challenge for their prediction using virtual testing. The application of virtual testing in understanding the mechanics of skin is progressing rapidly. Tepole and co-workers [151, 152] published their recent implementation of such an approach for skin growth, expansion and stretching. A typical

implementation of skin growth in a child is shown in **Figure 28** for increasing skin area. The authors developed a computational model, based on a nonlinear continuum mechanics, for stretch-induced skin growth during tissue expansion [151, 152]. Skin growth was multiplicatively decomposed into elastic and growth deformation gradient parts. The authors assumed that skin growth was characterized by irreversible, stretch-driven transversely isotropic process: captured solely using a scalar-valued growth multiplier called the in-plane area growth. Such a computational model serves as a virtual testing scheme for aiding reconstructive surgery in patients with congenital skin conditions or badly burned patients. The input for the model originate from microstructural information (often at cell-level) leading to a hyperelastic material model of the skin. The processes underpinning the skin behaviour – when subjected to loading by a tissue expander, as well as the recovery response (when the pressure loads are removed) - are reliably modelled using the above material model thus informing further clinical choices to both the patient and the doctor. Virtual testing here establishes a new paradigm for integrating the growth law of skin (originating from biological processes) with the mechanobiology (the influence of forces on the biology of skin) [153].

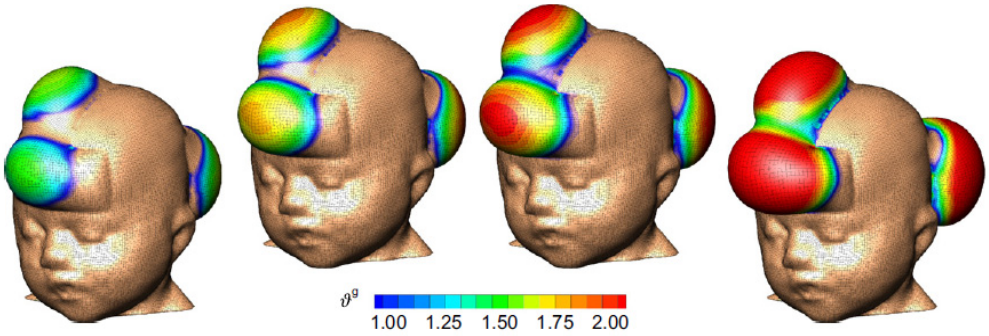


Figure 28: Illustration of different stages of simultaneous forehead, anterior and posterior forehead scalp expansion in a paediatric forehead reconstruction. The contour plot shows the changing skin area following skin expansion such that an initial skin area of 149.4 cm^2 grows to 251.2 cm^2 [154].

In order to study the mechanical properties of skin following aging, Magnenat-Thalmann and colleagues [148] also developed a skin modelling computational framework specifically dedicated to simulation of skin fold and wrinkle formation. The results from such a framework will inform the development of cosmetic products for reconstructive surgery of third-degree burn patients. Aging in skin was evident in the reduction in structure and mechanical properties of the skin: a consequence of alterations in the upper dermis of the skin. The computational skin model predicts reliably the folding capacity of the skin under transverse compressive loading. The skin was modelled as a multiscale

three-layered structure with each layer having different biomechanical properties. Results from this virtual testing of the skin confirm experimental data on skin wrinkling.

4.3.3 Collagens, Ligaments and Tendons

According to Reese and co-workers [31], collagens form the basic building block of ligaments and tendons. Collagens are hierarchically organized into complex structures that span multiple physical scales. Ligaments and tendons have a basic composition of water and fibrillar type I collagen. The observed macroscale behaviour is as a result of behaviour originating at micro- and meso- lengthscales respectively. For example tissue repair and growth results from fibroblasts and tenocytes: the latter being microscale constituents of skin, whose modifications will lead to mesoscale (repair and growth) changes. The exchange of information across the multiple lengthscales is difficult to establish using experimental approaches, hence the attraction of virtual testing to such studies. This review highlights some of the recent virtual testing implementations for multiscale analysis of collagens, ligaments and tendons.

Soft collagenous tissues are arranged in a highly hierarchical structure between the micro-, meso- and macroscale lengthscales [155]. The nanoscale consists mainly of molecules for collagen of type I. The microscale is composed of crimped periodic fibres and influence significantly the macroscopic mechanics of both regular (e.g. tendons) or irregular (e.g. skin) tissues [156]. The stress-strain response of most soft tissues is J-shaped distinguished by three different regions: *toe* (as a result of fibres microscopic crimp); *heel* (due to elongation of molecular kinks) and finally a *linear* region (due to stretching of the collagen triple helices. The *unified model* proposed by Maceri and co-workers [156] tracks the biomechanics of soft collagenous tissues from the nanomechanics of collagens to micromechanics of collagen fibres and finally predicting the macromechanics of unidirectional soft collagenous tissues. At the nanomechanics level of analysis, a nonlinear constitutive behaviour of the collagens was developed incorporating an entropic mechanism of collagen molecules and their corresponding stretching effects. At higher scales, crimped collagens were homogenized into unidirectional equivalent ones – accounting for both geometrical and material nonlinearities. The approach was successfully used to model the multidirectional behaviour of aortic media, using experimental inputs based on histological and morphological parameters of the test material. This approach is consistent with the principles of virtual testing for heterogeneous materials.

Laurent and colleagues [157] used virtual testing in the mechanical modelling of tissue engineering scaffolds of anterior cruciate ligament (ACL). The authors treated the ACL scaffold as a multi-layered braided structure with explicit modelling of the constituent fibres that make up the structure, as shown in **Figure 29**. The braided structure provides a network of pores adapted for tissue ingrowth [158]. Accurate model representation is central to replicating the expected mechanical

response of a typical ACL scaffold, hence resulting in computer-aided tissue engineering of ACLs. The multi-layer braided structure can easily be modified by changing the braiding angle, α number of fibre layers, *L* and the fibre diameter, *D*: all that influence stability of the restored knee.

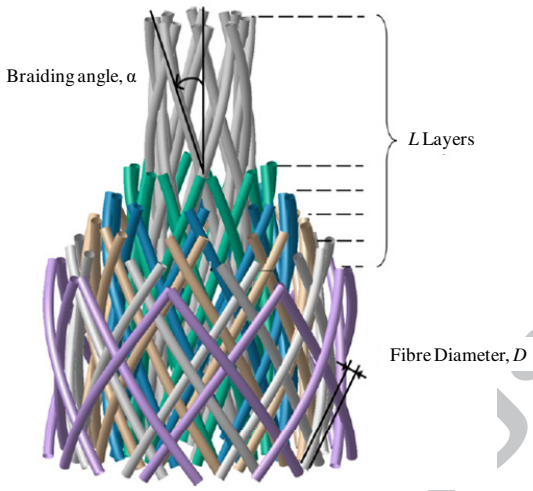


Figure 29: Architecture of an Anterior Cruciate Ligament multi-layer braided scaffold [157].

The microscale constitutive material model in each scaffold is a copoly(lactic acid-co-(ε-caprolactone)) (PLCL) – a copolymer. The fibre was modelled using a beam model and the stress-strain response was Hookean. Appropriate contact mechanics was incorporated into the virtual test model to account for contacts between fibres.

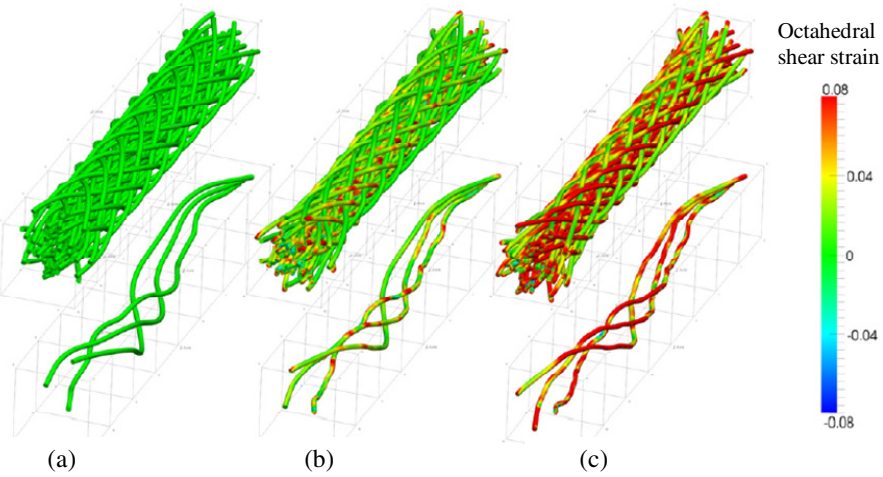


Figure 30: Contour plots showing octahedral shear strains on the surface of the scaffold and three selected fibres taken from the scaffold for (a) initial configuration (b) tension/torsion test (tension = 45°, stretch = 4.5%) and (c) tension/torsion test (torsion = 90°, stretch = 9%) [157].

Boundary conditions for the model are such that the ends of the fibres are imposed with tensile loading with the fibres allowed to re-arrange in response to the prescribed load cases. The sequence of

deformation response from initial configuration for a set of fibres and different levels of torsion and tension loading is given in **Figure 30**. Comparisons with experiments agreed well. The authors concluded the virtual testing approach is valuable for determining optimal tissue repair configurations[157].

4.3.4 Wood

Wood is a heterogeneous, anisotropic and hygroscopic natural composite material with high specific strength and stiffness[159]. Macroscopically, wood is orthotropic with: *longitudinal (L), radial (R)* and *tangential (T)* directions. A typical wood cell wall consists of cellulose, hemicelluloses and lignin. It is often composed of crystalline and amorphous regions [160]. The high stiffness results from the crystalline fraction while the flexibility results from the amorphous region. The non-crystalline region can absorb moisture and is subject to changing mechanical properties [161]. The highly multiscale structure of wood is illustrated in **Figure 31**.

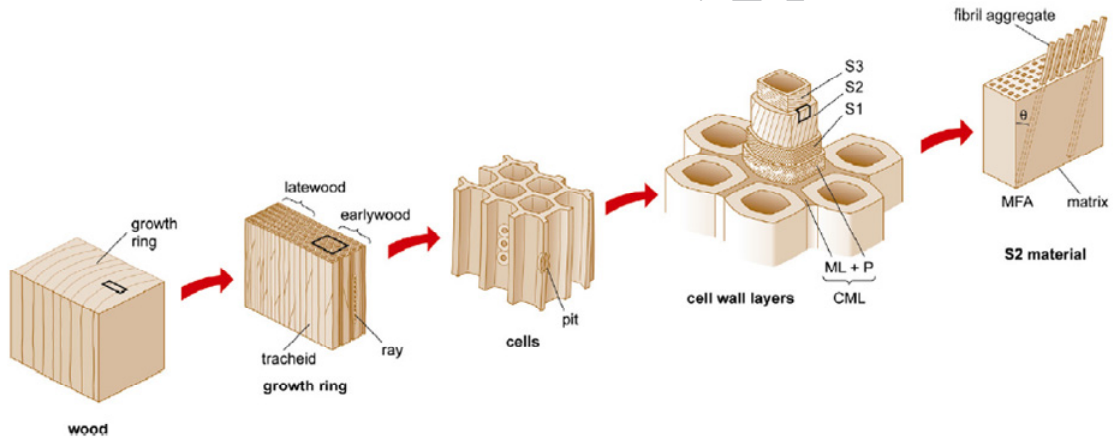


Figure 31: Illustration of the multiscale structure of wood [162].

Wood continues to be an important engineering material hence the need to develop better predictive tool to support more sustained commercial exploitation of wood. Recent commercial interests in wood as a design material of choice are driven mostly by environmental concerns, low costs, low thermal conductivity and very low electrical conductivity [159]. As a result, the understanding of the effects of microstructure on mechanical properties has become an active area of research. This is also an area where virtual testing approaches are useful in enhancing the applicability of wood in several engineering applications. This section of the review highlights some of the current virtual testing implementations for wood.

Virtual testing models of wood have been based on micromechanical modelling approaches. These were subdivided into: cellular models, homogenization-based models and discrete (composite, laminate) models [159, 163-165]. Each sub-division corresponds to a definite lengthscale of wood. A

typical cellular model of a *Nepalese wood* modelled by Qing and Mishnaevsky [159] was based on an idealized geometry of a honeycomb cell. Their study and others [110, 166-168] showed that the properties, shapes, and dimensions of the cell wall material determine the elastic moduli and strengths of wood.

Homogenization-based models exist for predicting the mechanical properties of wood. A typical example is that of Hofstetter and colleagues [169] which is a micro-elastic model for wood based on a four-step homogenization scheme. The model determines the properties by incorporating information at different lengthscales. At nanometres, hemicelluloses, lignin and water are all intimately mixed within a dynamic polymer network. Cell wall materials are modelled at the microscale as fibre-like aggregates of crystalline and amorphous cellulose within a polymer matrix. At the mesoscale, softwood was defined and modelled by cylindrical pores (lumen) and finally at the macroscale of about several millimetres, hardwood is modelled by larger cylindrical pores. This modelling approach allows for the incorporation of the moisture-dependent properties of wood.

Qing and Mishnaevsky [170] developed a virtual testing framework for understanding the influence of moisture, density and microstructure on hydroelastic and shrinkage properties of latewood. This framework used a 3D hierarchical finite element model of softwood cells represented as hexagonal-shaped tubes with multilayered walls as shown in **Figure 32**. Each cell sub-layer has distinct elastic properties obtained from unit cell models. The moisture effects on local elastic properties were modelled by representing the moisture effects by an equivalent temperature effect within ABAQUS^{TM} FEM framework. Following comparisons between numerical and experimental data, the authors concluded that the shrinkage of softwood increases linearly with moisture content possibly up to 25%. Shrinkage properties in the longitudinal direction were an order of magnitude lower than that in the transverse direction. The authors also reported that the microfibril angle affects the longitudinal Young's modulus of wood. Finally the wood density had a strong influence on the elastic properties of wood with the former increasing with the later in all directions.

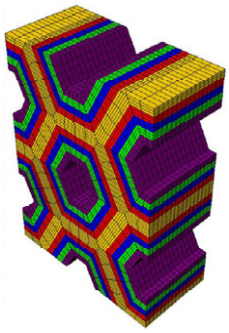


Figure 32: A 3D hierarchical RVE = of wood comprising hexagonal cells with each sub-layer having distinct elastic properties [170].

Saavedra Flores and co-workers [161] developed a multi-scale virtual framework for investigating the highly non-linear irreversible behaviour of wood cell-walls. The model was described as a finite strain three-scale model where the overall response of the cell-wall composite was obtained by computational homogenization of a *microfibril-RVE* of cell-wall material whose mechanical response prediction, in turn involves the computational homogenization of a *cellulose core-RVE* [161]. The framework reliably predicted (in comparison with experimental data) the following features of mechanical behaviour of wood cell-wall: viscous relaxation, stiffness recovery mechanism and hysteresis. The study observed that the inelastic yielding of the amorphous cellulose is the main driver to cell wall failure under straining. The authors concluded that the proposed virtual framework can inform further analysis of the dissipative response of wood and how microscale effects influence macroscale behaviour.

Finally, Rafsanjani and colleagues [162] also developed a computational model for investigating the hygro-mechanical behaviour of a hierarchical cellular material, in particular the growth rings of softwood. The authors used a two-scale micro-mechanics model imposed with robust homogenization techniques: accounting for material anisotropy of cell walls and geometry of cellular structure. The RVE unit cell is honeycomb and simulations were based on periodic boundary conditions. In comparison with experimental data, the model predicted reliably the mechanical properties of the test material as well as the swelling behaviour of a growth ring in transverse directions. Key conclusions from their work showed high tangential/radial (*T/R*) swelling ratio at the start of the growth ring in early wood which decreases along the relative ring position and becomes close to 1.0 in latewood. The opposite observation is the case for the elastic *T/R* ratio which initially is constant in earlywood and increases significantly in latewood.

5.0 THE STRUCTURE OF A VIRTUAL TESTING LABORATORY

Literature is awash with instances of pseudo-laboratories designed to replicate physical experiments [171, 172]. Such laboratories are simply software-based experiments designed for user interaction without physically attending laboratory sessions. The developmental efforts for such pseudo-laboratories are geared towards mimicking real experiments in feel, structure and setup. There is no consideration here for the mechanics of the materials under investigation. Such virtual laboratories are in order words augmented reality scenarios of the physical experiments. Examples of such laboratories are commonplace in undergraduate education. These are not the type of laboratories which this review paper is considering.

The aim of the virtual laboratory being discussed here is the investigation of the mechanics of heterogeneous materials; hence the focus will be on the underlining computational engines that drive the virtual laboratory. In developing such a virtual laboratory (VL), the core objective is always building a structure that is analogous to a physical laboratory. Traditional experiments involve test specimens, load cells and strain gauges, testing equipment and subsequent data reduction analysis. Similarly, a VL is designed such that the geometry of the test specimen is modelled as a representative volume element (RVE), and the measurements of forces and/or displacements obtained from calibrated load cells and strain gauges are comparable to 'boundary condition' inputs within a virtual laboratory. Material models are incorporated within the VL to simulate the behaviour of the test material. Such material models serve as the computational engines – incorporating the underlining physics of the heterogeneous material's response. Also, a numerical platform within the VL is synonymous to the test equipment used in real experiments e.g. the Instron machine. Such numerical platform consists of an FE solver, model development scripts, user-defined sub-routines, etc. Analogous to data reduction process is the whole range of post-processing activities of the VL. Model validation is the last process before results from VLs are stored in a results database. If comparisons between experimental data (where they exist) and numerical predictions are accepted, then data is logged in a results database, but if such comparisons are rejected, then further iterative and optimization processes are carried out until acceptable results are obtained. All these features of the phenomenological laboratory should be incorporated analogously within a probable VL as shown schematically in **Figure 33**. In the following paragraphs, examples of typical virtual laboratories will be presented to illustrate how their structure fit within the process flow chart identified in **Figure 33**.

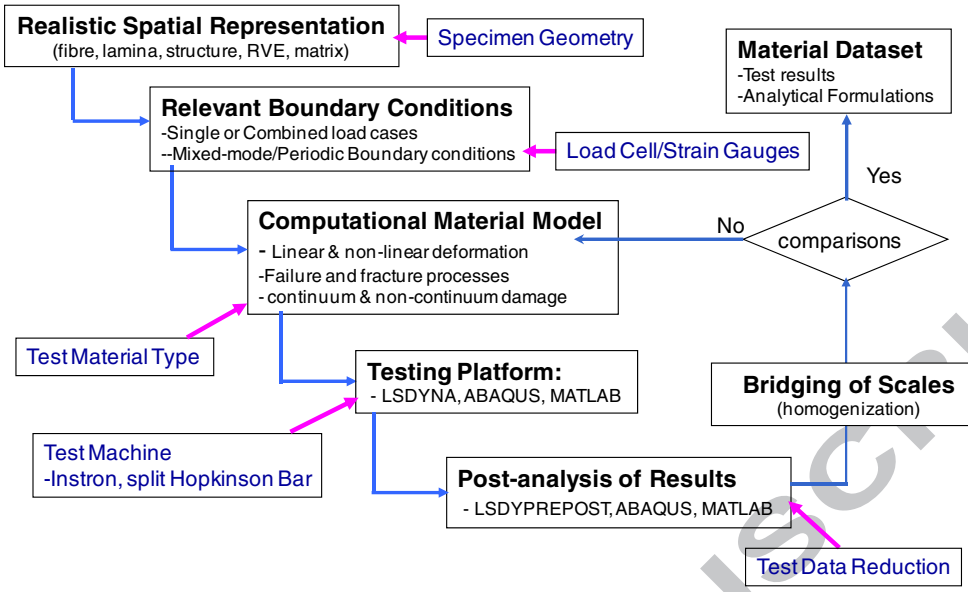


Figure 33: Process flow chart for a virtual laboratory.

One of the earliest implementations of a virtual laboratory is the *Virtual Test Facility* (VTF) by Caltech Centre for the Simulation of Dynamic Response in Materials [173, 174]. The VTF is defined as "*a problem-solving environment for full 3D parallel simulation of the dynamic response of materials undergoing compression due to shock waves.*" The VTF is a software environment designed for: (a) computation of effects of shock waves impinging targets (b) computation of dynamic behaviour of the targeted material and (c) validation of computations. The authors described their version of the virtual test facility as "*a federation of computational engines tied together and driven by a user interface.*" The computational engines were developed to implement the fluid- and solid-mechanics equations underlying the simulations. According to the process flow chart of Figure 2, the VTF capabilities range from experimental geometry generation (i.e. RVEs) to visualizing of simulation outputs. The flow chart for the VTF is given in **Figure 34**. A Python front-end is used for interpreting and inputting data for the VTF. The computational engines that drive the VTF are: solid mechanics, solid-fluid coupling and CFD solvers. Other sets of tools like the Nexus/Globus, Scalable I/O, etc were used for archiving and visualizing the resulting data.

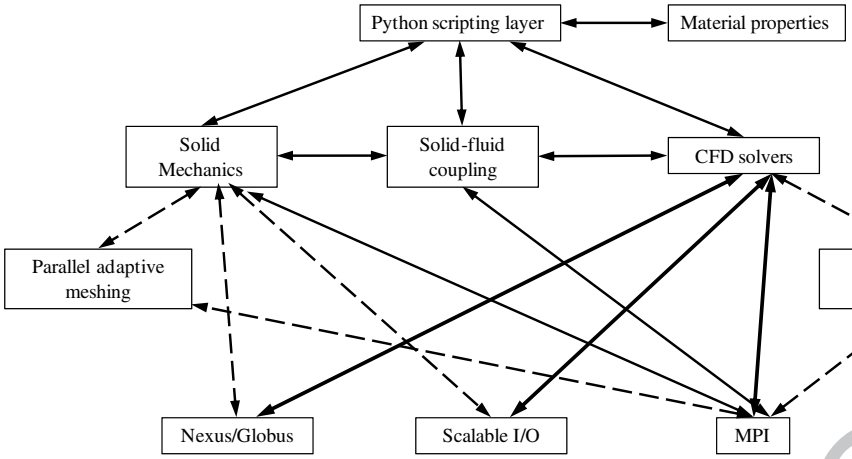


Figure 34: The Virtual Test Facility (VTF) software architecture [173].

Another virtual test laboratory was designed for concrete materials and described as the Virtual Cement and Concrete Testing Laboratory (VCCTL) [15, 76]. This virtual laboratory was developed as a multi-scale predictive tool for the cement paste (micrometres in size) and concrete (millimetres in size). According to the developers of this variant of the virtual laboratory, the goal was to "*reduce the number of physical concrete tests, whether for quality assurance or for expediting the research and development process"* [15]. In order to determine typical predicted properties of concrete, the VCCTL incorporates the underlining manufacturing processes (e.g. curing), constituents (e.g. cement, aggregates), and properties (e.g. volume fraction of aggregates, particle shape) of concrete. The schematic representation of the VCCTL is given in **Figure 35**.

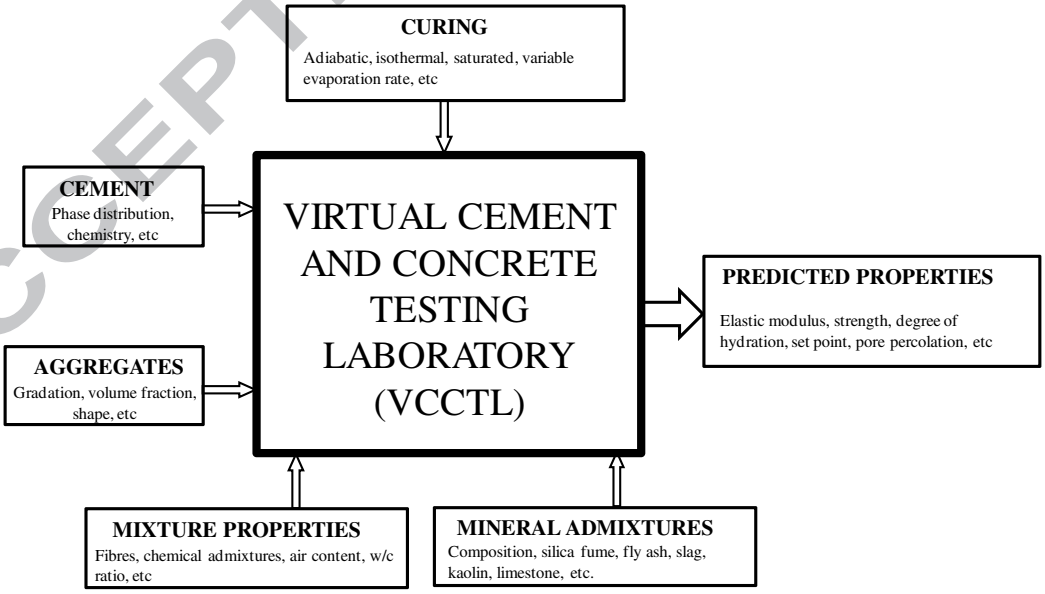


Figure 35: The structure of the Virtual Cement and Concrete Testing Laboratory [15].

Most recently, Okereke and Akpoyomare [11] developed a virtual laboratory for determining the holistic elastic properties of a unidirectional (UD) composite. The authors called the VL a virtual framework and it was described as: "*a multi-step implementation process ranging from the generation of realistic geometric models of a test composite to the prediction of all possible macroscale effective elastic constants*" [11]. The VL incorporated 3D RVEs of a typical UD composite with realistic spatial realization of the fibre inclusions; robust boundary conditions representative of physical tests and adequate homogenization techniques were used to bridge the scale between the macroscale validation data and microscale predictions of the 3D RVEs. The schematic representation of the virtual laboratory is given in **Figure 36**.

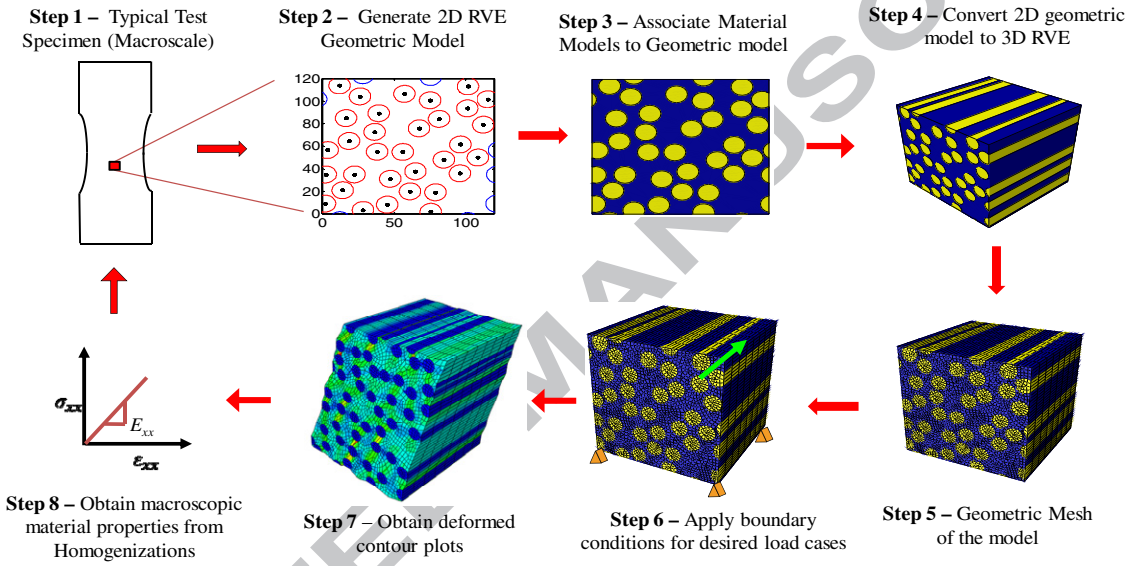


Figure 36: The component steps of a UD composite virtual framework [11].

Other comparable virtual laboratories have been developed in the last two to four years. For example Anderson and Rayfield [175] developed a virtual laboratory for exploring the mechanics of biological systems – in particular tooth morphology. In another development Llorca and co-workers [36] broadened their virtual testing argument by incorporating a virtual module capable of simulating the processing histories of test materials (e.g. curing, forming), to the traditional virtual testing scheme shown in **Figure 33**. This was illustrated using composite materials within a multi-scale scheme incorporating molecular dynamics and Monte Carlo techniques. In the authors' opinion the incorporation of virtual testing with virtual processing following molecular dynamics and Monte Carlo techniques should serve as a road map towards the realizing the goal of virtual tests replacing physical experiments. Zeng and Lu [176] espoused this road map in their review article, by detailing the virtual processing and multiscale modelling strategies across molecular, microscale, mesoscale and macroscale length and time scales, for polymer nanocomposites.

6.0 CHALLENGES TO FUTURE VIRTUAL TESTBEDS

The discussion of the different virtual testing frameworks for heterogeneous materials demonstrates the onerous challenges encountered in several aspects of virtual testing: (a) accurate geometric modelling (b) development of characteristic multiscale material models (c) choice of appropriate boundary conditions (e) development of robust homogenization techniques and finally (e) the challenge for validation of numerical predictions with experimental data. To date, some authors have implemented varying levels of complexities of some aspects of these challenges for their particular virtual testing framework. The objective will always remain the incorporation of the most realistic and robust variants of each of those challenges within a given virtual testing framework; and when this is done, the objective of such virtual tests replacing real experiments would be realizable.

However, even with the current level of development in virtual testing, further challenges remain that have not yet been considered in the development of virtual testbeds. This section of the review discusses these challenges with a view towards building a hypothetical structure of future virtual testing frameworks. The task of developing innovative solutions to address these challenges will constitute the research goals for next generation engineers and scientists.

6.1 Exploring beyond the design space

The objective of virtual testing is always to create a computational framework which can reliably predict known phenomenological responses of a given test material. This implies that a set of experimental data exists which any numerical prediction must be compared with in other to verify the reliability of such numerical predictions. Authors of existing virtual testing frameworks, described in section 5, always concluded with some form of validation of their numerical predictions. However, what happens for those constitutive responses that are difficult to replicate experimentally? In other words, if the design data does not exist for certain scenarios and it is crucial that understanding has to be developed for such scenarios, what will the engineer do? This is what the authors describe as *the challenge of exploring beyond the design space.*

Future virtual testing frameworks must seek to liberate the design space within which the test materials are used. This implies developing a framework which is *intelligent* and *intuitive* in its ability to predict behaviours of the test material where traditional laboratory experiments are not viable. Such framework will become a trusted design tool which will not only provide guidance on validated test cases but also those cases which only a numerical solution is possible.

6.2 Novel Materials and their architectures

Future virtual testbeds must be able to tackle the challenge of ever increasing developments of novel materials and their often complex architectures. Such complexity arises from their inherent heterogeneity or intricate architectural conformations. With the development of new materials and

architectures, experimental challenges arise; and therefore, such materials need to be modelled within a virtual testing scheme. In a recent report by the McKinsey Global Institute, the authors of the report [177] identified *Advanced Materials* as the 10th most significant advance that will transform life, business and the global economy, with a potential economic impact of $0.2 - $0.5 trillion in 2025. The report identified the following as leading candidates in this material revolution: graphene, carbon nanotubes, nanoparticles (e.g. nanoscale gold and silver), and other advanced and smart materials (piezoelectric materials, memory metals, self-healing materials). In particular, graphene presents an interesting modelling challenge. Graphene possess a two-dimensional lattice structure comprising a single layer of carbon atoms arranged in a honeycomb structure. Although it is the world's thinnest material, it is also the world's strongest material [178-180]. In the future, quite a lot of applications will be based around graphene due essentially to its diverse properties [181-184]. Future virtual testing frameworks must address the challenge of predictive modelling of the diverse properties of these advanced materials thereby tapping into the opportunities presented by these materials in many applications.

6.3 Virtual testbeds borne out of industry-academic collaboration

Most of the existing virtual testing frameworks described in this review have been developed in an academic community – with researchers working independently of inputs from industry. The explanation for this could be the need by academic researchers to simplify virtual testing into modules which can be solved without the complexities that practical scenarios present. However, if the target of virtual testing being a replacement for practical experiments is to be achieved, then virtual testbeds must address practical scenarios. The driver for the modelling problem would have to come from practical industrial challenges. It should be acknowledged that the length scale of industrial problems is usually at macroscale and most academic implementations of virtual testing are at microscale – with a view towards informing macroscale behaviour. Therefore, this review demands that future virtual testbeds must begin to address practical industrial challenges – even grappling with the challenges of the length scale differences. This approach demands a closer interaction between industrial and academic partners. A major advantage to this approach is the incorporation of a feedback mechanism between the two collaborators which will lead to enhancements of current versions of the virtual testbeds. The HYPERCON project [15, 76] which led to the development of the VCCTL virtual testing framework developed for concrete materials is an ideal case study where enhanced collaboration between academic and industrial partners was in place. This trend should be adopted in future virtual testing frameworks.

6.4 Integrating coupon-level virtual test results into structural level designs

Traditionally, aerospace engineers have always used coupon level experiments to determine mechanical properties required for aircraft certification tests [185]. Coupon-level tests (tensile, compression, shear, etc) are a window into the mechanical behaviour of the test material. However, the structural response of the material is always different from the coupon-level behaviour [186-188]. This discrepancy was identified by Cox and Yang [32] as a consequence of the lengthscale effects: manifest in using either a bottom-up or top-down modelling approach within a virtual testing framework. Acar and co-workers [185] further investigated the scale effects by assessing the number of coupon and future element tests (in aero industries) required to comprehensively describe the distribution of failure stress on aircraft structural parts. Therefore, it is essential that the mechanics of relating lower scale properties at structural scales has to be developed. Future virtual testbeds must also address this challenge in order for such testbeds to replace structural level experiments.

6.5 Computational mechanics at structural level are still very elementary

Computational mechanics principles required at structural level of analysis, for many classes of heterogeneous materials, are at a rudimentary stage of development. For the purpose of this article (refer to **Figure 1**), structural levels are defined as the next length scale above the macroscale for many classes of materials. For example, for composite materials, the structural scale can span from tens of centimetres to many metres. Therefore, classic computational mesomechanics and macromechanics approaches fall short of dealing with prediction of structural responses. For a biomaterial like the bone, the structural length scale can be representative of the complete human form. At such scales, distinctions exist between the mechanics of the femur, tibia, ulna, skull, vertebra, etc. Some of the approaches already discussed in sections 5.1 and 5.3.1 for composites and bone respectively cannot deal with the distinctions evident at structural scales.

According to Llorca *et al* [36], the challenge of structural scale computational mechanics stems mainly from the computational cost required to predict structural response based on microscale inputs. Although rapid progress has been made in the last decade computationally, many desktop computations of structural problems are still limited by excessive demands on micro-processor capabilities and system memory as well as convergence of high mesh density problems.

There are few works on asymptotic homogenization for structural mechanics [189, 190]. However, computational homogenization techniques (required for virtual testbeds) are too simplistic: often extending microscale analyses into macroscale conclusions with simplifying assumptions [191, 192]. The later technique should achieve efficient bridging of scales between micro, meso- and macroscales and structural length scales: with microscale variations affecting structural response. The physics underpinning such bridging, without excessive '*smearing'* of the structural response, has not been properly understood. Edmans and co-workers [193] recently published a feasible approach for dealing

with computational homogenization at structural scales. The authors' nonlinear computational homogenization was based on: (a) introducing a linear operator that maps the smooth part of a small-scale micro-displacement field to that of the large-scale and (b) use of trace operator to impose boundary conditions on an RVE. The approach still suffers from *smearing* and *loss of refind details* at the structural scale. Therefore, future developers of virtual testbeds should tackle this challenge. Unless this is done, improvements from microscale to macroscale may continue as they are at the moment, but the gulf in understanding between the macroscale and structural scales will continue to limit the widespread applicability of virtual testing frameworks in industrial problems.

6.6 The stochastic of microstructure argument

A pertinent question that faces developers of a virtual testbed is: should one use a microstructure reconstruction (based on say tomographic images) or apply selected topological parameters to create regularized numerically-generated RVEs? The use of tomographic images often gives realistic reconstructions of the microstructure but the computational cost of generating the virtual domains are excessive and extra deployment may not be justified. Therefore, only few existing virtual testbeds have used numerical reconstructions based on topological parameters of the microstructure. Stig and Hallstrom [10] developed a 3D virtual domains for textile composites on the principle of numerical reconstructions. A typical example is the work of Rinaldi and co-workers [52] who used statistical data from micro-tomographic images to reproduce a virtual textile composite. Stig and Hallström [10], on the other hand, used regularized numerically-generated (TexGen-based) 3D virtual domains for their simulations.

The challenge facing future virtual testbed developers is the definition of a virtual domain that is not regularized in composition and distribution. This is what the authors describe as the *stochastic of microstructure* argument. The statistics of the microstructure is a key consideration for defining an acceptable virtual domain. It is known that a range of nonlinear microscale processes that influence failure, damage evolution, etc. of many test materials arise from the stochastic distributions of the microscale. Okereke and Akpoyomare [11] used a statistical descriptor to determine the suitability, within a virtual testbed, of a numerically-generated 3D RVE of a UD composite. This and *perturbation-based homogenization approaches* [194] give localized stochastic effects. However, realistic virtual domains should incorporate both localized and far field stochastic of microstructure effects. Some of the emerging approaches that are worth considering include: those of Lamon *et al* [82], Basaruddin and co-workers [195], Williams and Baxter [196].

6.7 The quest for high-fidelity experimental data

The current approach of justifying the suitability of a given model (or virtual testbed) for prediction of mechanical response of a given test material relies appreciably on experimental data. Blau and co-workers [197] argued that although this approach is conceptually sound, yet there exist limitations to

the approach. A key limitation is the *paucity of high quality experimental data* [197]. In other words, the quality of the experimental data available to the virtual testbed developer will significantly affect the validity of predictions from the testbed. Garboczi *et al* [76] also argued that high quality experimental data are central to the virtual testing process. Such data are derived from careful characterization of the test materials. The challenge for future virtual testbeds is a continued practice of designing innovative experiments that explore several multiscale aspects of a given test materials. Extensive research efforts are required for experimental characterizations. In other words, any possible advancement in computational methods will always be limited by any regression in the experimental process.

One particular area where innovative experiments have to be designed is the microscale. If evolution of cracks from numerical processes are to be validated using experimental data, then new experimental modalities have to be designed which will assess such microscale or often times nanoscale processes. In this way, predictions at the microscale can be validated: establishing confidence that microscale models can be used as inputs for a higher scale analysis. At the moment, the theoretical basis behind microscale processes has been used solely to establish confidence in predictions. However, there is a growing community of researchers working on innovative experiments to investigate and validate microscale models. Some of the promising approaches that need to be investigated further include: Banks-Sill *et al* [198] in situ microscale tensile tests, Szczepanski and co-workers *microscale fatigue experiments*[199]; Chan *et al* [203] microscale plastic deformation experiment in microforming processes[200]; Kimberly and co-workers' [204] dynamic response of micro-machined beams; Katsamenis *et al* [201] lamellar level cortical bone load bearing characterization. All these approaches describe an objective process of understanding the microscale behaviour of heterogeneous materials.

7.0 CONCLUSION

This paper has addressed the emergence of virtual testing frameworks for heterogeneous materials. Virtual testing as used in this work refers to the application of computational methods to the mechanics of heterogeneous materials. In many cases, the computational platform used has been mainly a finite element tool (ABAQUS, ANSYS, MIMIC, etc.). However, computational methods as defined in this communication are not limited to only finite element analysis. Virtual testing, as used in this study, focuses on tracking the effects of microscale variations/modelling on macroscale response. This is different from aero-industry definition of virtual testing where coupon-level experimental data is extrapolated to define structural level response.

The work established initially the implication of lengthscales in the development of virtual testbeds. Lengthscales are central to the discussion of heterogeneous materials as these materials can be either considered heterogeneous (at a sub-scale) or homogeneous (at a higher scale). Depending on the selected lengthscale definition, the underlining theoretical framework must be appropriately tailored to suit that lengthscale. The approach for relating sub-scale, macroscale and even structural level response is dependent on the lengthscales chosen for the virtual testing framework. Therefore, clear definition of all applicable lengthscales is essential when developing a virtual testbed.

This study also explored the structure of existing virtual testbeds with a view to identifying the common features that are evident within a given framework. It was observed that it is essential that virtual testing frameworks must reflect analogously the structure of a physical laboratory experiment. In other words, it is important to define a specimen geometry (referred to as an RVE within the testbed), incorporate a test material (represented by a material model), decide on adequate boundary conditions to represent the results from strain gauges and load cells, etc. Finally, as physical testing is always carried out on a test machine, a virtual framework lives on some numerical platform which can include but not limited to FEM environment, MATLAB, Python programming, etc. The key component of the virtual testbed is the computational engines which comprise mostly the numerical tools created to explore the mechanics of the test material on a numerical platform. Typical examples of current virtual testbeds and their distinctive features were also presented.

The main objective of this review was to highlight existing virtual testing frameworks for different classes of heterogeneous materials. Here, several frameworks have been discussed ranging from various classes of composite, biomaterials and cellular materials. A multiscale analysis involving analyses at nanoscale, microscale, mesoscale and macroscale were consistently implemented across the different test materials considered. The study specifically assessed the suitability of the proposed virtual testbeds towards replacing physical experiments, which in the authors' opinion, remain the main objective behind every virtual testing scheme.

The paper concluded with a reflection on what future virtual testbeds need to possess for them to be realistic substitutes to practical experiments. The specific challenges that remain unresolved were identified and recommended as research directions that future developers of virtual testing frameworks must address if the ideal of such virtual laboratories replacing and/or complementing physical experiments is to be realized. Such challenges span from accurate definition of model geometry; advances in structural and stochastic mechanics; better collaboration between industry and academia – to inform the virtual testing development - and finally the necessity for generating high quality validation data at not only macroscale but also microscale. Although there is great promise in existing virtual frameworks, exciting challenges remain which will continue to occupy developers of virtual testbeds. Just as Oden *et al* [1] predicted, when the above challenges are addressed and next generation virtual frameworks designed, radically new *computational tools* would be developed. Such tools will be able to predict the gamut of linear, nonlinear and post-yield thermo-mechanical responses of heterogeneous materials: without recourse to physical experiments. Above all, such tools will make it possible to open up the design envelope currently limited by a few sets of experimental data points.

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