PARTICLE-BASED MODELLING OF THE GEOMETRY AND MECHANICAL BEHAVIOUR OF TEXTILE REINFORCEMENTS

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1 Introduction

Mechanical loading imposed on RTM / VARTM / RFI preforms during PMC manufacturing compacts the preforms along the normal to their plane, shears them in-plane, and induces bending and other deformations. This alters the configuration of yarns in preforms: elastic, time-recovered and permanent deformations are imparted to the yarns leading to yarn flattening, nesting and inter-layer packing. All these factors lead to complex preform geometry at the scale of yarns and textile unit cells [1, 2].

The constitutive properties of the dry preforms, their processing properties such as their permeability to liquid resins, and the material properties of the PMC parts made from these preforms are influenced by this complex yarn configuration, to varying extents. For example, the in-plane permeability to resin or the interlaminar shear strength of the PMCs may be strongly affected while the in-plane stiffness or through-thickness thermal conductivity may not be influenced significantly [3-7]. Prediction of changes in preform configuration induced during the manufacturing of PMC parts is useful in terms of providing accurate predictions of the processing and performance properties of preforms and PMC parts.

Particle-based computational methods constitute a powerful general numerical tool for simulating the large-strain mechanical behaviour of non-homogeneous dry preforms, accounting for their detailed configuration at the yarn scale. In this work, particle-based simulations of fibre assemblies were used for locating fibre positions and quantifying fibre interactions that minimize the total strain energy stored in fibre assemblies during PMC manufacturing. In a given simulation step and under constant boundary conditions, iterative calculations based on the Metropolis algorithm [8] using specific interaction functions bring the fibre assembly from an arbitrary initial state of strain energy to a state of minimum strain energy. Then, displacements are applied at the boundaries of the textile domain and the iterative process is repeated. Simulations show that the compaction and shear of fibre assemblies lead to a shift in fibre positions but also to a change in yarn shapes and contact configuration; furthermore, this change is time-dependent. A parallel is drawn between the iterative process and the time-dependent behaviour observed with textiles made of perfectly elastic fibres, hence modelling the time-dependence is an integral part of the method with only one scaling parameter needed for adjusting numbers of iterations to time [9, 10].

This work features simulations leading to the prediction of configurations and to the identification of the constitutive behaviour for various textile assemblies, as well as experimental validation trials. Simulations of the compaction, time-dependent relaxation and in-plane shear are reported. In a first step, simulations are reported featuring lesser numbers of larger fibres made of different materials; these simulations are replicated in validation trials. In a second step, application of the simulation method to assemblies featuring larger numbers of smaller fibres for which it would be impractical to replicate each fibre individually, is introduced through an expansion algorithm presented herein. The particle-based method utilizes discrete mechanics as an alternative to traditional mechanics of continua. The present implementation enables intricate geometric modelling of preforms at the yarn scale as well as the realistic modelling of the constitutive behaviour during PMC manufacturing.

2 Modelling methodology

In the basic version of the modelling method, fibres are represented as a series of discrete spherical particles with diameters equal to the fibre diameter. The relative positions of individual particles in a
series collectively describe the fibre geometry. A modified Metropolis algorithm \[8\] with Boolean decision function is used for iterating particle positions towards configurations of lower strain energy. Once a stable level of strain energy is reached or a set number of iterations are done, boundary conditions are changed to reflect on-going compaction or in-plane shear and the iterative procedure is repeated.

Any relative displacement between particles that results either from changes in boundary conditions or from iteration under stable boundary conditions produces changes in strain energy. Changes in strain energy which can be associated with axial tension, axial compression or bending stresses; fibre torsion is neglected. Changes in strain energy result from i) relative displacement between particles within a single fibre leading to changes in intra-fibre strain energy, and ii) fibre deformations resulting specifically from interactions between neighbouring fibres, leading to changes in inter-fibre strain energy. All terms are detailed below.

The intra-fibre strain energy term \(U_A\) arising from axial tension/compression is a function of fibre material's Young's modulus \(E\), fibre cross-section area \(A\), and distances between 2 particles \(l_{ab}\) and \(l\) under and without loading respectively. Equation 1, Fig. 1. Inter-fibre bending strain energy \(U_B\) is calculated from the fibre material's Young's modulus \(E\), fibre second moment of area \(I\) for circular fibres and angle defined between three successive particles, Equation 2, assuming an initially straight fibre as represented by angle \(\pi\).

\[
U_A = \frac{AE}{2E}(l_{ab} - l)^2
\]

\[
U_B = \frac{EI}{l_{cd} + l_{de}}(\pi - \psi)^2
\]

Contact forces between curvilinear fibres within a fibre assembly such as a yarn may be calculated using Gutowski’s compaction model \[13\]. The selection of this function was investigated and validated \[14\]; simulations and experimental trials showed it to be well-suited for particle-based modelling of textiles. Gutowski’s compaction model states that instead of being perfectly straight, individual fibres within yarns are wavy; \(\beta\) is a fitting parameter in Gutowski’s function either evaluated by microscopy or fitted to experimental results. In the model is assumed that \(l_{min}\), the minimum distance between two particles, is equal to \(2r\).

From Gutowski’s model the inter-fibre strain energy term is calculated by integrating force over distance for the displaced particle interacting with surrounding fibres; for a particle separated by distance \(l_{ij}\) with \(l_{min} < l_{ij} < l_o\) strain energy is calculated as:

\[
U_G = \int F_{ij} \cdot dx = \int \frac{192EI}{\beta^3} \cdot \frac{(l_o - l_{ij})^3}{(l_{ij} - l_{min})^3} \, dl_{ij}
\]

where \(l_o\) is the initial distance between particle centres. Gutowski’s model is equivalent to the beam bending equation with reducing span; it has been used successfully \[13, 15, 16\] in many occurrences.

An important physical parameter in the system is friction, which partially restricts fibres from slipping relatively to each other. Whilst conservative strain energy terms associated with elastic loading may be calculated for a given static configuration, non-conservative friction losses occur only as the fibre assembly goes from one configuration to other. Friction also contributes to hysteretic losses observed experimentally in deformed textiles, most notably for relaxation and in-plane shear.
Two approaches in managing friction may be considered in particle-based modelling. In a direct approach, normal forces between pairs of contacting fibres are determined at every contact point. Displacements at all contact points in the fibre assembly are also calculated. Knowing these forces and displacements, a total energy loss associated with fibre friction between two configurations is obtained. This direct approach requires highly computational iterative work due to number of contact points involved. Also, a proper value of the coefficient of friction must be introduced from trials, the determination of which is not trivial.

The alternative indirect approach proceeds as follows. In the absence of friction, contacting fibres slip freely relative to each other and resulting configurations are dictated only by the ensuing reduction in total elastic strain energy stored in the assembly at a given fibre volume fraction, as discussed above. Upon iteration, generally any tentative configuration that reduces the elastic strain energy stored in the textile is accepted as the new configuration on an ongoing basis. In the presence of friction, fibre slippage is impeded and as a result, additional energy must be expended for evolving towards configurations corresponding to same fibre volume fraction as for a system without friction. This is integrated in the algorithm by altering the strain energy threshold conducting to a tentative configuration being accepted upon iteration. The energy balance will only remain favourable if final configurations with lower strain energy levels are accepted. A percentage is applied on the strain energy in the initial state, which remains constant through the entire simulation. As a result, at lower fibre volume fractions when fewer contacts are present, friction generally does not have a major effect. However with increases in fibre volume fraction and number of contacts, strain energy differences resulting from small displacement have a more significant effect as reasonably expected.

3 Experimental

Initial experimental validation trials were conducted using plain weave fabrics made of yarns containing 30 monofilament Nylon 6/6 fibres, with 5 mm yarn spacing in both directions. Diameter of the Nylon 6/6 fibres was measured at 299 ± 1 μm, Table 1. An Instron 4482 universal testing frame equipped with a 1 kN load cell was used for compaction, relaxation and in-plane shear experiments. Young’s modulus of Nylon 6/6 fibres was measured at 1.05 ± 0.02 GPa. Characteristics of the fibres and textile samples appear in Table 1.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Number of samples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fibre diameter</td>
<td>299 ± 1 μm</td>
</tr>
<tr>
<td>Fibre density</td>
<td>1.172 ± 0.001 g/cm³</td>
</tr>
<tr>
<td>Initial v_f of textile</td>
<td>22 ± 2.3 %</td>
</tr>
<tr>
<td>Surface density of textile</td>
<td>0.103 ± 0.001 g/cm²</td>
</tr>
<tr>
<td>Number of fibres in yarn</td>
<td>30</td>
</tr>
</tbody>
</table>

4 Compaction

Virtual samples in compaction simulations featured yarns made of 30 virtual Nylon 6/6 fibres with 300 μm diameter, woven into plain weave textiles; results reported with fibres made from other materials are reported elsewhere [14]. Yarns, single textile layers and double textile layers were simulated. Fibres in most samples featured 60 particles along their length; some samples featuring longer fibres were also simulated for probing any effect of fibre length.

Compaction was simulated by progressively reducing the domain height h. Fibres located near the upper boundary were displaced accordingly; the total strain energy was minimized iteratively under constant boundary conditions. The number of iterations was unchanged in each compaction step but it changed between different simulations, replicating different compaction rates. Displacements during compaction and load retrieval steps were set to 0.1 μm and compaction pressure P was recorded as a function of h at each 100 steps by summing the vertical components of forces applying on the horizontal boundaries. Maximum particle displacement or random walk step was set to 1.0 μm. Gutowski’s parameters were β = 200, v_p = 0.28 and v_d = 0.79 for Nylon 6/6 fibres as identified in previous work [14]. Values of the fibre volume fraction v_f were obtained in two ways. v_f calculation method 1 proceeds by
identifying fibres crossing a rectangular plane and adding individual cross-section areas, accounting for any angle between the normal to the plane and the local fibre direction. Plane height corresponds to domain height and plane width is, at most, the minimum width that encompasses all fibres. The sum of section areas is then divided by the plane area. \( \nu_f \) calculation method 2 proceeds by calculating the volume of all fibres whilst neglecting compaction of individual fibres as per Hertz’ model [11], and dividing by the volume of the smallest rectangular cuboid encompassing all fibres.

Fig. 2 shows two steps in the compaction of a single layer of plain weave textile. Simulations featured textile domains with 4 yarns in each direction and 16 crossovers; no lateral boundaries were used. Values of \( P \) and \( \nu_f \) were calculated over a smaller domain in in-plane dimensions as shown in Fig. 2 and extending over the domain thickness.

Simulation results appear in Fig. 3 along with experimental validation results. Experimental trials were conducted by compacting a single layer between two parallel platens mounted and aligned in the Instron frame, Fig. 4. Upper platen dimensions were 40 mm x 40 mm. Effect of any platen assembly deformation was measured from dry compaction runs performed with no textile sample placed between the platens, and removed from the raw compaction data from tests where textiles were compacted. Samples were aligned at 45° from platen edges to reduce any orientation edge effect.

Following simulations performed of a single layer, double layer stacks of the same textile were also simulated, firstly with perfectly aligned yarns and secondly with yarns that were perfectly staggered in both directions Fig. 5. These latter simulations showed the ability of the particle-based modelling environment to replicate nesting. During the compaction phase of the double layer stack with perfectly aligned yarns, pressure increased from lower fiber volume fractions compared with the stack featuring yarns that were perfectly staggered Fig. 6. Yarn cross-sections in the center of the layers appear for both cases in Fig. 5.
5 Relaxation

Simulations of relaxation were conducted, where virtual samples were compacted and held to constant thickness. A reduction in pressure ensued from the iterative process; iterations were effectively associated with time. The simulation series featured cases where the numbers of iterations between each compaction step were set at $2 \times 10^5$, $5 \times 10^5$ and $10 \times 10^5$ respectively, Fig. 7. The maximum pressure was set at 0.5 MPa.

Fig. 7. Compaction and relaxation of virtual single layer plain weave textiles subjected to different number of iterations with the same target pressure

As seen in Fig. 8 small numbers of iterations corresponding to very fast compaction lead to higher levels of relaxation after the compaction phase, with a maximum relaxation value of about 50% from maximum pressure observed for the parameters selected. The larger reduction in pressure observed at higher rates, after compaction, is a consequence of pressure building-up more quickly at lower $v_f$ during the compaction phase. In view of experimental results presented below, higher numbers of iterations are more appropriate in replicating experimental results for the parameters selected in this work.

Experimental relaxation trials were conducted using compaction rates of 2.0, 1.0 and 0.5 mm/min, Fig. 9. Maximum target pressure was set to 0.45 MPa. Textile samples were compacted to the maximum pressure and then held to the thickness reached at that pressure, enabling relaxation. Relaxation periods were kept constant at 360 seconds in all 3
6 In-plane shear

The area covered by a textile submitted to in-plane shear reduces, leading to an increase in \( v_f \) under constant thickness. Inter-yarn spacing defined perpendicularly to warp yarns and to weft yarns both decrease, eventually leading to contact and lateral compaction of the yarns. Shear can also increase yarn crimp as yarns get thicker, with less inter-yarn space available for interlocking. Finally, as crossovers are no longer defined by yarns crossing at 90°, the yarn sections effectively rotate around the yarn axis. All these effects can lead to tensioning of the yarns and fibres within them.

In-plane shear simulations based on the algorithm described in section 2 were performed, that replicated articulated frame in-plane shear testing. Ends of each individual fibre were positioned within planes representing the edge of the frame. In all simulations, all fibres in the balanced fabrics had the same initial free length between edges. In-plane shear was induced by progressively reducing angle
$2\theta$ defined between the two upper edges corresponding to the articulated frame, Fig. 11.

Fig. 11. Simulation of 16 crossovers plain weave textile undergoing in-plane shear in articulated frame configuration

Different sets of boundary conditions may be imposed for attaching fibres to the frame edges during in-plane shear simulations. Here, fibre were modelled as attached to the frame edges through pivots that can rotate freely and may be displaced in the plane of frame edges, within the initial area defining the associated edge plane. The height and width of all boundary areas corresponds to the initial dimensions of the edge planes, and they remain unchanged during simulations.

Fig. 12. Nylon 6/6 textile sample undergoing in-plane shear test in articulated frame

Experimental trials were conducted using an articulated frame that featured four aluminum edges connected together by four ball bearing pivots. The upper and lower pivots were connected to the Instron 4482 universal testing frame with pin-type load cell mounts. Displacement speed was set to 1 mm/min. As the traverse of the universal testing frame pulled the upper and lower pivots away from each other at a constant rate, the frame angle $2\theta$ decreased at the hinge and the textile sample was sheared, Fig. 12.

In-plane shear results are typically reported using shear angle $\alpha$ which is a macroscopic measure of shear defined at the scale of the sample and corresponds to the departure from the initial 90° angle defined between the two upper edges of the articulated shear frame. It can also be viewed as the departure from the nominal 90° angle between the warp and weft orientations. Angle $\alpha$ is initially 0° and increases upon shearing. Values of $\alpha$ during a test are determined from the vertical displacement of the top hinge, Equation 4, where $d$ is hinge displacement from its initial position and $L_{\text{frame}}$ is the length of shear frame edges.

$$\alpha = 90^\circ - 2\cos^{-1}\left(\frac{\sqrt{2L_{\text{frame}}+d}}{2L_{\text{frame}}}\right)$$  \hspace{1cm} (4)

Results for in-plane shear force normalised with respect to edge length as a function of shear angle showed close results to the experimental trials, Fig. 13; only minor differences between experimental trial and simulation were observed.

Fig. 13. Normalized shear force $F_N$ as function of shear angle $\alpha$ for simulation and experimental trial

Textile thickness was probed as it is an important parameter to processing and performance of technical textiles and PMCs. Thickness was defined as the vertical distance between the lowest and highest particles found within a domain as it is
sheared. Fig. 14 shows that the unrestricted thickness of the simulated textile increased under in-plane shear, in a manner consistent with behaviour generally reported in the literature. For the simulated textile, thickness starts increasing mostly around a given value of the shear angle, with a generally linear trend beyond that value. The decrease in spacing leads to reorganization of the fibres within yarns and translates into fibre network reorganization at higher numbers of iterations, comparable to experimental trials using lesser compaction rates.

The two major components of intra-fibre strain energy in EA-fibres are the axial tension/compression term and the bending term, as discussed above for physical fibres. Fundamentally, the expansion algorithm aims at replacing \( n \) real, smaller physical fibres of radius \( r \) with \( N \) EA-fibres of larger radius \( R \), where both the total volume of fibre material and volume of the domain remain the same. Both fibre assemblies should have the same axial stiffness and bending stiffness at the same fibre volume fraction. In an EA-fibre, strain energy in axial tension/compression \( U_A \) is a function of Young's modulus \( E \), which is not changed when going from physical to EA-fibres. Strain energy also relates to the distance between particles which will be larger than for physical fibres in typical models.

The strain energy stored in an EA-fibre subjected to pure bending is defined by the equivalent Young's modulus \( E \), second moment of inertia \( I_{EA} \) and segment length \( L \). Bending of each physical and EA-fibre is reasonably assumed to take place independently around their individual neutral axes, and so \( I_{EA} \) is affected only by the diameter increase. Therefore, \( I_{EA} \) is altered for EA-fibre diameter in the expansion algorithm. As stated above, when replacing a large number of physical fibres by a smaller number of EA-fibres within a physical domain of identical dimensions, it is desired to maintain a constant value for \( v_f \). Given the fact that the fibre volume fraction and so the volume of material must stay the same for both cases with physical and EA-fibres:

\[
v_{f_{EA}} = v_{f_r} \tag{5}
\]

\[
N.R^2 = n.r^2 \tag{6}
\]

Meanwhile, for both cases of simulations with physical fibres and EA-fibres Equation 9 needs to be satisfied on the grounds that bending one EA-fibre around a given radius should require the same amount of strain energy as bending \( n/N \) physical fibres having the same length \( L \) and made of the same material, around the same bending radius. Therefore the following relations must be satisfied:

7 Expansion algorithm

Applying the particle-based modelling method described above to textile reinforcements with yarns featuring thousands of fibres was investigated, leading to the development of an expansion algorithm described in this section.

Through the expansion algorithm, one may generate curves representing the constitutive behaviour of such reinforcements using simulations featuring less fibres in an otherwise unchanged domain. Each fibre modelled for usage in the context of the expansion algorithm represents a number of actual physical fibres with different dimensions and properties; the constitutive behaviour of these larger fibres is adapted so as to replicate the behaviour of a number of actual fibres. The larger modelled fibres are labelled herein as EA-fibre. EA-fibres have a circular cross-section, the diameter of which is larger than that of the individual physical fibres that each EA-fibre represents. Material properties are altered appropriately as highlighted below. Other elements of the simulation environment remain essentially unchanged.

Fig. 14. Textile thickness and yarn center spacing as a function of shear angle \( \alpha \)
\[ I_{EA} = \sum I_r \]  \hspace{1cm} (7)
\[ \frac{\pi r^4}{4} = \frac{n}{N} \cdot \frac{\pi r^4}{4} \]  \hspace{1cm} (8)
\[ N \cdot R^4 = n \cdot r^4 \]  \hspace{1cm} (9)

where, again, the moments of inertia in bending of the physical and EA-fibres are labelled as \( I_r \) and \( I_{AE} \) respectively.

It is seen that Equation 9 is incompatible with the above statements and Equation 6. The solution adopted consists in using a different value of Young's modulus for EA-fibres that is specific to the strain energy bending term only and is not used in the axial tension/compression term. The increase in total bending stiffness when going from \( n \) fibres of readies \( r \) to \( N \) fibres of radius \( R \) is effectively too large, and so the solution consists in dividing Young's modulus \( E_m \) by \( n/N \) in the bending strain energy term only. As such, reducing the modulus by \( n/N \) will lead to the same bending strain energy being imparted as if bending the same mass of physical fibres extending over the same length.

Textile reinforcement used in manufacturing composites and modelled using the expansion algorithm feature EA-fibres, the centrelines of which are further apart than those of the more numerous physical fibres that they aim to represent within the same domain. Forces between individual pairs of fibres must be increased as they are less numerous, both to compensate higher distances in Gutowski's model and the smaller number of fibres contacting say the top surface and contributing to pressure. This is done by altering Gutowski’s model as shown below.

As Gutowski’s model uses the distance between the centrelines of two neighbouring fibres as its main input parameter, a relation between this distance, the number of fibres in a domain, and the domain size must be established towards the aforementioned objective. The simpler development proposed here is based on parallel fibres; it is worth noting that it remains widely applicable to more complex cases as fundamentally the expansion algorithm applies to yarns as opposed to textiles.

The relation is established by reasonably assuming as a starting point that parallel fibres align in a triangular or hexagonal configuration as this

maximises the distance between neighbouring fibres at a given \( v_f \), hence minimising any strain energy term associated with lateral compaction of the yarn. Whilst insightful geometric arguments can be made and demonstrated about boundary conditions leading to networks of parallel fibres that are more stable for constant \( v_f \) and domain size if the domains are relatively wider, for larger numbers of fibres this boundary effect becomes negligible. The main conclusion enabled by the above assumption is that the number of triangles that may be defined from lines normal to the centrelines of neighbouring parallel fibres tends toward double of the number of fibres. So given a domain size and a number of fibres, the dimensions of the triangles defining fibre positioning in a network of parallel fibres which will lead to a state of lower strain energy may be obtained, and so the distance between 2 neighbouring fibres can be calculated directly. The ratio of the distance to \( v_f \) stays constant for different numbers of fibres hence direct scaling can be applied. Distances are multiplied by a factor \( y \) in Gutowski's model, and so multiplying forces by \( y^2 \) constitutes the needed scaling. The only parameter that changes for a network of EA-fibres is inter-fibre distances, and \( f \) which can be processed as explained above for bending. As a result, dimensions are multiplied by \( y \) equal to reduction factor \( n/N \) and Gutowski's equation is modified as follows for EA-fibres:

\[ F_G = \frac{192E_l}{\beta^3} \cdot \frac{\gamma(l_{a-iij})}{\gamma^2(l_{ij}-l_{min})^2} \cdot d_{lij} \]  \hspace{1cm} (10)

The above increases forces generated within EA-fibres by \( y^2 \) to obtain same forces generated as with the actual number of physical fibres. Reducing the number of fibres does not change the way in which the proportion of fibres contacting the top surface to the total number of fibres in the assembly evolves as compaction proceeds.

8 Conclusion

In this work, a particle-based modelling method enabling the accurate modelling of the geometry and constitutive behaviour of textile assemblies was developed. Simulation results were validated experimentally for single layer textiles and some cases of multi layer textiles. Validation work shows that the particle-based modelling method replicates
reality very well. The modelling enables better understanding of the behaviour of the textiles and the deformation that they undergo as they are loaded.

Single layers of plain weave textiles featuring multiple plain weave unit cells were simulated for compaction, relaxation and in-plane shear. Results shown for example in Fig. 3. for compaction of the single layer matched experimental results well. Double-layer stacks of the same textile were also simulated for compaction behaviour, firstly with perfectly aligned yarns and secondly with yarns that were perfectly staggered in both directions. These double layer simulations aimed at investigating the ability of the particle-based modelling method at replicating nesting. In the staggered case, higher \( v_f \) results at lower \( P \) due to the shifted layers. Results for relaxation and in-plane shear also investigated the configuration of the textiles in detail, and good correspondence with experimental trials was observed.

The introduced expansion algorithm makes it possible to use less, larger fibres for predicting the mechanical behaviour of textiles featuring large numbers of smaller fibres, such as textile reinforcement used in manufacturing composites.

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**References**