A Continuum-Microscopic Model of Fibrous, Heterogeneous Media with Dynamic Microstructures

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Abstract

Creating accurate, macroscopic scale models of microscopically heterogeneous media is computationally challenging. The difficulty is increased for materials with time-varying microstructures. Common modeling approaches for heterogeneous media include purely continuum-based models and homogenization methods. However, these methods tend to blur the inhomogeneities of the material that can influence local mechanical properties. Continuum-microscopic (CM) models are a class of methods that incorporate microscopic information into faster macroscopic models of the medium. CM methods have been used for heterogeneous media with static microstructures. This article presents an extension of a basic CM algorithm to model heterogeneous media with time-varying microstructures. Fibrous media are chosen as a class of materials upon which to test the algorithm. Information from the material's microstructure is saved over time in the form of probability distribution functions (PDFs). These PDFs are then extrapolated forward in time to predict what the microstructure will look like in the future. Keeping track of the microstructure over time allows for accurate computation of the local mechanical parameters used in the continuum-level equations. The model was tested on a generic fibrous material with randomly oriented and crosslinked fibers. Results show that the mechanical parameters computed with this algorithm are similar to those computed with a fully-microscopic model. Errors for continuum level variables in the 5-10% range are deemed an acceptable trade-off for the large savings in computational expense offered by this algorithm.

1 Introduction

Due to the discrete nature of matter, multiple spatial and temporal scales exist in many natural phenomena. These different scales can be governed by unique physical laws and the matter itself may be characterized differently at each scale [14, 17]. For illustrative purposes, consider an ideal gas. At the scale where individual gas molecules are observable, molecular dynamics can be utilized to describe the motion of these discrete elements [25]. At a larger scale where the molecules can no longer be distinguished from one another, the gas can be characterized as a continuum and modeled by the Euler equations of fluid dynamics [23]. Molecular dynamics could still be used at this larger scale to model the motion of the gas, however doing so would incur a large computational expense due to the large number of molecules in the system [1, 14, 30]. The continuum assumption allows for fast computations and is a valid choice for materials with homogeneous or regularly patterned discrete structures [1, 19]. However if the medium has a heterogeneous structure, a purely continuum based model will likely fail to capture the true mechanical properties and behavior of the system [11, 30].

Creating accurate and efficient models of heterogeneous media is computationally challenging. A class of models that shows promise for modeling such materials is known as continuum-microscopic (CM) methods. These methods combine a detailed model of the material's microstructure with a faster continuum model of the medium [14]. CM models have thus far been employed for materials whose microstructure is known or can be consistently approximated by an assumed configuration [14, 17, 22]. However, there are many examples of media that do not conform to these assumptions. Materials such as fibrous composites often have complex, non-uniform, discrete structures that deform and rearrange in response to applied forces [12, 38].

In this article, a novel CM model is presented to model heterogeneous media with dynamic microstructures. This model is able to retain memory of a material's microstructure over time so that local mechanical properties induced by changes in the microstructural configuration [35] can be accurately computed and passed on to the continuum equations throughout the simulation. The method is based on statistical sampling and the generation and extrapolation of probability distribution functions for the microstructure data.

After a presentation of pertinent background information, the new algorithm will be described. Its utility will then be demonstrated on an example fibrous composite system.

1.1 Continuum-Microscopic Models

CM methods combine the modeling of two scales (length, time, or both) usually governed by different physical laws into one algorithm [14]. The general idea behind CM methods is to utilize information obtained
from short evolutions of a very detailed model of the material to update or predict information for longer evolutions of a less detailed model where presumably computations can be done more efficiently [14]. The main CM methods include the Heterogeneous Multiscale Method (HMM) [13], Adaptive Mesh and Algorithm Refinement (AMAR) method [17] and the Equation-Free Method (EFM) [22]. In HMM there are typically two numerical schemes: one at the continuum level (e.g. a discretized conservation law) and one at the microscopic level (e.g. a system of molecular dynamics equations). The continuum model requires the computation of numerical data such as fluxes, forces, or mechanical parameters in order to advance. The microscopic model computes this missing information and passes it to the macroscopic model so that it can move forward. HMM has been applied in many scientific areas such as gas kinetics [37], fluids [31] and elasticity [1]. AMAR combines the ideas of grid refinement with the utilization of different equations at different refinement levels. Adaptive mesh refinement is used to better resolve a problem’s solution in an area of the domain. If the refinement changes the spatial scale by several orders of magnitude, the material’s description and governing physical laws may also change. The physical laws of this finer scale are used to update the variables in the refined area. The results are then utilized to update the solution on the overlying coarser grid. AMAR has been demonstrated for modeling shock waves and fluid shear [17]. EFM has the same goal as HMM to improve the solution of a continuum level problem by using microscopic scale information. The difference is that in EFM the continuum level equations are never explicitly advanced. The microscopic equation solutions are used to predict what the continuum variables will be at the next macroscopic time step. EFM has been applied to numerous subjects including population dynamics [6], disease evolution [10], peptide folding [21] and chemical reactions [27].

The basic steps of each of these CM algorithms are:

1. Create a microscopic instantiation of the system.
2. Advance the microscopic system a short number of time steps until the data values reach a quasi-state of equilibrium, or until enough data has been collected to discern a pattern of behavior.
3. Average the microscopic data and use it to update the continuum level model
4. Advance the continuum level system one large time step
5. Repeat steps 1-4

A schematic of this process is shown in Figure 1.

As stated in the introduction, CM models have thus far been utilized under the assumption that the material’s microstructure is known or can be reasonably approximated by a known distribution function (e.g. a uniform or normal distribution of the discrete elements) [14, 17, 22], making Step 1 of the process simple to perform. However, in materials like those described in the next section, their microstructures are highly heterogeneous and experience many changes and fluctuations over time, thus their microscopic configuration is generally unknown [11]. The method presented in this article extends the basic CM algorithm to model these types of materials.
1.2 Fibrous Composites

A class of materials known as fibrous composites will be utilized as a test case for this new algorithm. Composites are comprised of two or more materials with different mechanical properties [20]. Fibrous composites specifically refer to media composed of fibers embedded in a matrix material [33] or fibers entangled together in a network [34]. Examples include fiberglass [33], fabrics [11], paper [9], various engineered metal composites [12], and biological materials such as the cell cytoskeleton, cartilage, and connective tissues [2]. At a macroscopic scale these materials are often simulated with purely continuous models [3, 15] or with models that utilize homogenization methods [19, 26, 28]. However use of these techniques has come into question due to these materials' inhomogeneous microscopic structures [11].

CM models have been utilized for modeling heterogeneous media that obey one of the following assumptions: (1) the heterogeneities are assumed to be periodic [12, 16], (2) AMAR was utilized for a small region of the material, while the rest of the medium is assumed to be homogeneous [17], (3) the highly heterogeneous microstructure is known from the beginning and does not change during the simulation [30]. Many of the materials mentioned above have non-periodic, time-varying heterogeneous structures throughout their entire domain. For such materials, the instantiation procedure in Step 1 should produce a microstructure that represents a configuration the original microstructure could have evolved to if it had been simulated for the full time interval. Current CM models do not retain information about the material's microstructure from time step to time step and thus have no way of making an informed prediction of the microscopic configuration at future points in time. The model presented here can instead make predictions of future micro-states based on past micro-states.

2 The Macro and Micro Models

2.1 Macroscopic Model

A generic, fibrous material with randomly oriented fibers will be the test case for this model. At the macroscopic level this material is viewed as a continuum whose deformation is captured by the three-dimensional linear elasticity equations. This equation set includes six independent equations of motion derived from the time derivative of the infinitesimal strain tensor: \( \epsilon = \frac{1}{2}(\nabla u^T + \nabla u) \) where \( u \) is the displacement vector. Three more equations are acquired by Newton's Law \( F = ma \) for the three Cartesian directions. The equation set is closed by a constitutive law of the form:

\[
\sigma = C \epsilon
\]

where \( \sigma \) is the Cauchy stress tensor and \( C \) is the stiffness tensor [24]. \( C \) contains the material’s mechanical properties. It is here where the microscopic model will come into play, since these properties vary with space and time for heterogeneous media.

For the example in this article, the macroscopic domain will be a rectangular region that has dimensions 10 x 100 x 1 units. Physically, this may represent materials like a strip of fabric, a metallic fibrous composite beam, or a section of plant stem. This elastic material is attached to a wall at its left edge and will have stress applied to its right edge (see Figure 2). The domain is discretized into 1 x 1 x 1 unit grid cells for the numerical solution of the elasticity equations. Within each grid cell a microscopic scale model of the material is created. As the microstructure deforms due to applied stresses, its average mechanical properties will change and it is these varying parameters that will be periodically passed to the macroscopic constitutive law (Equation 1) to keep it up to date. In Step 4 of the general CM method, the elasticity equations are numerically advanced via a wave propagation algorithm [24, 29]. One side note before proceeding to the microscopic model: though the linear elasticity equations are used, the fact that the constitutive law varies with time introduces piecewise non-linearity to the problem, expanding the realm of possible applications.

2.2 Microscopic Model

Each three-dimensional grid cell in the macroscopic domain is assigned an initial microstructure of an interconnected fiber network. The fibers will be modeled as one-dimensional spring-like objects, and will be
2.2.1 Step 1 (First Initialization)

Begin with a three-dimensional grid cell with dimensions: \([x_{\text{min}}, x_{\text{max}}] \times [y_{\text{min}}, y_{\text{max}}] \times [z_{\text{min}}, z_{\text{max}}]\). To set up the initial network, \(n\) fibers are laid in the grid cell. This is done by placing one endpoint \((x_0, y_0, z_0)\) inside the block: \(x_{\text{min}} \leq x_0 \leq x_{\text{max}}, y_{\text{min}} \leq y_0 \leq y_{\text{max}}, z_{\text{min}} \leq z_0 \leq z_{\text{max}}\). The second endpoint \((x_1, y_1, z_1)\) is assigned by choosing: (1) a length \(L\) for the fiber using a Gaussian distribution centered around a mean length \(L_0\), (2) a direction vector \((x_{\text{dir}}, y_{\text{dir}}, z_{\text{dir}})\) established by uniform random number generation. The second endpoint is thus computed by: \(x_1 = x_0 + Lx_{\text{dir}}, y_1 = y_0 + Ly_{\text{dir}}, z_1 = z_0 + Lz_{\text{dir}}\). If this endpoint falls outside the block, the endpoint is revised to be the intersection point of that fiber with the cell wall through which it crosses. This fiber is flagged as attached to the wall, which will be important for when the block is deformed (to be explained shortly). The \(n\) fibers are assumed to be at their equilibrium lengths in this initial state, however strains could be assigned to each fiber if desired.

Crosslinks between fibers are established next. This is done by taking each fiber pair and finding the shortest distance between them. If this distance is below a certain threshold value, then a crosslink has a probability \(P\) of forming. A random number generator is used to pick a value \(x \in [0,1]\). If \(x < P\) a crosslink forms and is added to the system as a new short fiber connecting the two original fibers. Figure 3 shows an example grid cell containing a crosslinked network.
2.2.2 Step 2

If the grid cell walls move due to some imposed strains, the fiber network will react to the change. Natural systems tend to move towards an equilibrium state. From thermodynamics theory this state is characterized by maximum entropy, or equivalently minimal energy [7]. The fibers in the microstructure can be moved by solving an energy minimization problem. Mechanically, the fibers are treated as spring-like objects, thus their total potential energy is given by:

\[ U = \sum_{j=1}^{m} \left[ \frac{k_j}{2} (L_j - L_{j0})^2 \right] \]  

(2)

where \( k_j \) is the spring constant and \( L_j \) and \( L_{j0} \) are the current and equilibrium lengths respectively of fiber or crosslink segment \( j \). The current length \( L_j \) is found using the segment’s current endpoints:

\[ L_j = \sqrt{(x_j^1 - x_j^0)^2 + (y_j^1 - y_j^0)^2 + (z_j^1 - z_j^0)^2} \]

The values \( x_j^1, y_j^1, z_j^1, x_j^0, y_j^0, z_j^0 \) are the variables of the energy function in 2. A necessary condition for a minimum of 2 is that:

\[ \frac{\partial U}{\partial x_j^1} = 0, \quad \frac{\partial U}{\partial x_j^0} = 0 \]
\[ \frac{\partial U}{\partial y_j^1} = 0, \quad \frac{\partial U}{\partial y_j^0} = 0 \]
\[ \frac{\partial U}{\partial z_j^1} = 0, \quad \frac{\partial U}{\partial z_j^0} = 0 \]

for all internal fiber segments \( j \). (Endpoints of fibers attached to a grid cell wall, move with that wall and are fixed during the energy minimization procedure.) These partial derivatives produce a large nonlinear system of equations which is solved via an iterative, gradient search algorithm [5]. Once a position of minimal energy for the network has been found, the evolution proceeds to the next microstep.

2.2.3 Step 3

Once a sufficient number of microsteps have taken place, an updated set of mechanical properties for the block can be computed. This fibrous material is assumed to be isotropic. (Materials of this nature are likely non-isotropic, however the fact that the mechanical properties are updated periodically, lessens the restrictive nature of an isotropic assumption.) Under this assumption, the stiffness tensor \( C \) contains two independent parameters known as the Lamé coefficients, which can be recast as the shear and Young’s moduli of the material. An estimate of the Young’s modulus \( E \) of the fiber network can be obtained by solving a least squares problem for the following three equations: \( \sigma_{ii} = E \epsilon_{ii}, \ i = 1, 2, 3 \). Stresses \( \sigma_{ii} \) are calculated by first computing the sum of Hookean forces in the \( i \) direction of all fiber segments attached to the two walls with normals in the \( i \) direction. The total force is then converted to a stress by dividing by the area of the wall. The strain \( \epsilon_{ii} \) is computed using the displacements of the block from equilibrium. Once \( E \) has been estimated, the shear modulus \( \mu \) is found utilizing established relationships involving the Poisson ratio and bulk modulus of compressibility [24]. These moduli are then used to compute the Lamé coefficients to update \( C \).

As a demonstration of the changes in mechanical properties that can occur at the microscopic level, consider a one block network under an increasing, uniaxial, extensional strain. The two walls with equations of plane \( x = x_{\text{min}} \) and \( x = x_{\text{max}} \) will be moved outward a distance \( \Delta x \) during each microstep (see Figure 4). The Young’s modulus of the network was computed after each microstep and is also plotted in Figure 4. This fiber network exhibits strain hardening. As the network is stretched, the fibers tend to align themselves in the direction of strain to minimize their stored energy. This creates a more parallel set of fibers which increases the Young’s modulus of the network. These results are corroborated by other computational models of fiber networks [4, 9] and has also been demonstrated experimentally [8, 36].
Figure 4: (A) Original block (solid line) under an extensional strain (dashed line) in the x direction. (B) The Young’s modulus versus strain curve for a box of crosslinked fibers under an extensional strain.

Figure 5: A histogram of fiber orientation angles initially and after several microsteps during which the network is uniaxially, extensionally strained. The distribution shifts toward smaller angles as the fibers align themselves with the axis of strain.

3 Microscopic Reinstantiation

After the continuum level equations have advanced a large time step, the microstructure must be recreated so that updated mechanical parameters can be computed. The uniform distributions used to lay down the fibers initially cannot be used in future CM cycles because the microstructure has changed. Evidence of this is shown in Figure 5. The distribution of one of the two orientation angles of the fibers is shown before and after the network is extensionally strained.

In order to recreate the network at a future point in time, a prediction of the distribution of fiber orientation angles and strains will be needed. To accomplish this task, each fiber’s two angles $\theta$ and $\phi$ that define its direction in 3D space, and its strain $\epsilon$ are collected during each microstep of Step 2. Non-parametric probability distribution function (PDF) estimation techniques such as kernel estimation are used to approximate the underlying PDFs of the collected data sets for each microstep [32].

Three single variable PDFs $f(\theta)$, $g(\phi)$, and $h(\epsilon)$ cannot be used to describe the data because $\theta$, $\phi$ and $\epsilon$ are not independent (see Table 3). A joint PDF $F(\theta, \phi, \epsilon)$ should be estimated. However, to avoid the computational expense of multivariate PDF estimation, extrapolation and data regeneration, a different method was devised. The correlation coefficient $r$ between angles $\theta$ and $\phi$ is very low compared to the $r$ values between each angle.
Table 1: Correlation Coefficients between fiber orientation angles and strain

<table>
<thead>
<tr>
<th>Variable 1</th>
<th>Variable 2</th>
<th>Correlation Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\epsilon$</td>
<td>$\theta$</td>
<td>0.51</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>$\phi$</td>
<td>0.39</td>
</tr>
<tr>
<td>$\theta$</td>
<td>$\phi$</td>
<td>0.071</td>
</tr>
</tbody>
</table>

Figure 6: The strain of a fiber is saved into an angle pair bin (based on its two orientation angles). Once all strains have been stored in these bins, a mean and standard deviation is calculated for the data within each bin pair. These values are then used to create a normal distribution for the strains in each bin pair.

and the strain, thus single variable PDFs $f(\theta)$ and $g(\phi)$ are created for the two angles. The PDF for the fiber strain is established as follows. The range of $\theta$ is $[-\frac{\pi}{2}, \frac{\pi}{2}]$ and the range of $\phi$ is $[0, \pi]$. Each range is divided into $m$ bins of equal length $\frac{\pi}{m}$: $[-\frac{\pi}{2} + \frac{\pi}{m} i, -\frac{\pi}{2} + \frac{\pi}{m} (i + 1)]$ for $\theta$ and $[\frac{\pi}{m} j, \frac{\pi}{m} (j + 1)]$ for $\phi$ with $i = 0..m - 1, j = 0..m - 1$. Fiber $k$ has orientation angles $\theta_k \in [-\frac{\pi}{2} + \frac{\pi}{m} i, -\frac{\pi}{2} + \frac{\pi}{m} (i + 1)], \phi_k \in [\frac{\pi}{m} j, \frac{\pi}{m} (j + 1)]$ for some $i, j$ bin pair. Fiber strain $\epsilon_k$ is recorded in bin $i, j$. Once all fiber strains have been binned, a mean $\mu_{i,j}$ and standard deviation $\sigma_{i,j}$ of strain data in each bin pair $i, j$ is computed and used to construct a local normal distribution $N(\mu_{i,j}, \sigma_{i,j})$ of strains. These local distributions are put together in a global piecewise distribution for the fiber strain. During reinstatement, fiber $k$ is assigned two angles $\theta_k, \phi_k$ from $f(\theta)$ and $g(\phi)$, and its strain is assigned using the following distribution:

$$H(\epsilon) = N(\mu_{i,j}, \sigma_{i,j}) \quad \text{when} \quad \theta_k \in [-\frac{\pi}{2} + \frac{\pi}{m} i, -\frac{\pi}{2} + \frac{\pi}{m} (i + 1)], \phi_k \in [\frac{\pi}{m} j, \frac{\pi}{m} (j + 1)]$$

Figure 6 gives a visual representation of what is being done.

As an initial test of this data collection procedure, the original network with $n$ fibers was simulated from time $t_0$ to $t_p$ ($p$ microsteps). The PDFs generated at time $t_p$ by the above method were then used to create $M$ new networks at time $t_p$. The Young’s modulus of the original network at $t_p$ was compared to the average modulus of the $M$ networks at $t_p$. This test was done for increasing $n$. By the law of large numbers, as the number of fibers is increased the relative error between the Young’s moduli of the original and new networks should decrease [18]. Preliminary results did not show convergence, with the new networks consistently coming out with elastic moduli about 10% lower than the original network. The source of the problem was identified as the energy minimization. An energy correction algorithm was developed to solve this problem and is described in the next section.
3.1 Energy Correction

At $t_p$ when microscopic data is collected, the original network is in a state of minimal energy. When a new network is instantiated at $t_p$, it has different crosslink connectivity than the original network. It is likely not in a minimal energy state upon instantiation, and thus settles to a lower energy state when the energy minimization is applied. Lower energy translates to lower elasticity moduli. Figure 7 gives a visual description of what is happening.

The goal is to create a new network with stored energy $U_0$ (energy of the original network at $t_p$) that is also in a state of minimal energy. The entropy maximization problem of thermodynamics finds the equilibrium state of a system with maximum entropy $S$ constrained to have energy $U_0$ [7]. Due to the equivalence of the principles of maximum entropy and minimum energy, the solution to the $Max(S)$ problem will have energy $U_0$ and be in a state of minimal energy. In statistical mechanics, the entropy is defined as: $S = k_B \ln \Omega$, where $\Omega$ is the total number of possible equilibrium states of the system and $k_B$ is Boltzmann’s constant. For simple systems with few components, an expression for $S$ can easily be established. It is difficult to do so for complex systems such as the fiber network in this example, thus a modified extremum problem back in the context of energy minimization is formulated. The goal is to have both $U(X) = U_0$ and $\nabla U(X) = 0$ be true for the new network. To guarantee the creation of a network that fulfill both criteria, an algorithm based on the concepts of a root-finding, bisection method was developed.

First, two angles and a strain $\epsilon_i$ is assigned to each fiber via the method described previously. Energy minimization is then applied. Typically the resulting total energy $U_1$ is lower than the desired $U_0$ value. If $U_1 < U_0$ then this energy state is marked as a lower bound for the bisection method. To create an upper energy bound, begin with the same initial fiber configuration and strain assignment $\epsilon_i$. However, modify each $\epsilon_i$ as:

$$\epsilon_i^{new} = K \epsilon_i$$  \hspace{1cm} (3)

where $K$ is a constant greater than 1. This will raise all the strains of all the fibers by the same percentage. The energy minimization is then run on this system to find its final energy state $U_2$. If $U_2 > U_0$ then an
Figure 8: Several steps of the energy correction algorithm. The line is the target energy value $U_0$. The cross data shows the application of the energy minimization procedure to the same system with different initial strain states.

<table>
<thead>
<tr>
<th>Number of Filaments $n$</th>
<th>Relative Error $(E - E_0)/E_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>0.13</td>
</tr>
<tr>
<td>500</td>
<td>0.0592</td>
</tr>
<tr>
<td>1000</td>
<td>0.03</td>
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<td>2000</td>
<td>0.00512</td>
</tr>
<tr>
<td>5000</td>
<td>0.004509</td>
</tr>
</tbody>
</table>

Figure 9: The relative error in Young’s modulus between the new networks and the original network for increasing numbers of fibers in the 3D networks. Strains were assigned using the binning method and energy correction algorithm described above. The graph shows the relative errors in a log-log plot. Data is shown with the dashed lines and the solid line is the line of best fit through the data. The convergence rate is found to be close to linear at -1.15.

upper bound has been found. If $U_2 < U_0$ then process 3 is repeated with a larger $K$ value. Once an upper and lower bound have been found, bisection can be used to zero in on a $K$ value that will result in a network whose minimal energy state has total energy $U_0$. Figure 8 shows several steps of the process. This method has been shown to produce the same results as the entropy maximization problem for simple systems [39].

Results of the convergence test comparing the original Young’s modulus to the new networks’ average modulus using this method are shown in Figure 9. The relative errors approach the 0.5% range and the rate of convergence is approximately linear at -1.15.
### Table

<table>
<thead>
<tr>
<th>Number of MicroSteps $p$</th>
<th>Relative Error at $t_n$ $(E - E_0)/E_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.1682</td>
</tr>
<tr>
<td>10</td>
<td>0.0813</td>
</tr>
<tr>
<td>15</td>
<td>0.0615</td>
</tr>
<tr>
<td>20</td>
<td>0.0217</td>
</tr>
</tbody>
</table>

Figure 10: The relative error in Young’s modulus found for increasing numbers of microsteps $p$ used in the PDF extrapolation algorithm to reinstantiate a new network at time $t_n$, in table and log-log plot form.

#### 3.2 Extrapolation

The algorithm will now be extended to reinstantiate networks at later points in time $t_n > t_p$ utilizing the data collected during microsteps $t_0-t_p$. PDFs $f(\theta)$ and $g(\phi)$ are constructed for the angle data at each microstep $t_j$, $j = 0..p$, thus for clarity they will be denoted as $f(\theta, t_j)$ and $g(\phi, t_j)$. The goal is to understand how these PDFs evolve over time in order to predict their shape at $t_n$. To do this $N$ evenly spaced angle values $\theta_i = -\frac{\pi}{2} + \frac{\pi}{N}(i - 1)$ and $\phi_i = \frac{\pi}{N}(i - 1)$ with $i = 1..N$ are chosen. Their function values at time $t_j$ are computed as $f(\theta_i, t_j)$ and $g(\phi_i, t_j)$ with $i = 1..N$ and $j = 0..p$. This gives $p + 1$ coordinate pairs per angle $i$ for both $\theta$ and $\phi$:

\[
(t_0, f(\theta_1, t_0)), (t_1, f(\theta_1, t_1)), ..., (t_p, f(\theta_1, t_p))
\]

\[
(t_0, g(\phi_1, t_0)), (t_1, g(\phi_1, t_1)), ..., (t_p, g(\phi_1, t_p))
\]

Least square approximation functions denoted $\hat{\Theta}_i(t)$ and $\hat{\Phi}_i(t)$ are created for the data in 4-5 for each $\theta_i$ and $\phi_i$. To create the predicted PDF of angle $\theta$ at time $t_n$, the coordinate pairs $(\theta_i, \hat{\Theta}_i(t_n))$ for $i = 1..N$ are interpolated using cubic splines. The same is done for angle $\phi$. Similar procedures are done to extrapolate forward in time, the mean and variance of the strains in each angle bin pair, as well as the total energy of the system. This extrapolated information is then used in the reinstantiation procedure in Step 1.

To test this extrapolation algorithm, data was gathered for microsteps $t_0-t_p$ of a network of fibers placed under an external strain. PDFs of the data were predicted for a future point in time $t_n$ using the method described above. $M$ new networks were instantiated from these PDFs at time $t_n$. The average Young’s modulus of the $M$ networks at $t_n$ was compared to the Young’s modulus of the original network at $t_n$, (which was fully simulated to $t_n$ for this comparison). The results for various numbers of microsteps $p$ are shown in Figure 10, and as one would expect the error decreases for increasing $p$ values. The new networks were then strained for an additional $q$ steps from $t_n-t_{n+q}$, to qualitatively compare the evolution of their moduli to that of the original network. Figure 11 shows the Young’s modulus of the original network and that of several reconstructed networks for two different $p$ values.

#### 4 Full Simulation Results

The rectangular macroscopic domain in Figure 2 was utilized for a full scale test. The novel CM model was applied to simulate the deformation of the domain under an extensional strain. The results from this simulation will be denoted as the microscopic reinstantiation (MR) case. As a means for comparison, a full
Elasticity Moduli vs. Strain for Original and Reconstructed Networks

Figure 11: Two plots depicting the original elasticity modulus versus strain (thick line) and the elasticity modulus versus strain of reinstantiated networks (thin lines) after a leap forward in time has occurred. Each graph shows a different leap size (denoted by the two yellow circles)

microscopic (FM) simulation was also done, where the original fiber network in each grid cell was simulated for the full time interval and no reinstatement was done. Error assessments will be made by comparing MR and FM data in the same grid cells.

Figure 12 shows examples of the comparison in Young’s moduli of the FM versus MR simulations for four blocks in the domain. The two curves take on the same general trend in each block. Time plots of macroscopic stress variable $\sigma_{xx}$ for the two cases are shown side-by-side in Figure 13. The results are qualitatively similar. The average relative error over time in $\sigma_{xx}$ over a subset of all grid cells is shown in Figure 14. In general the errors are in the range of 5-10%.

There is an approximately 50-75% reduction in computational time with the MR simulation versus the FM simulation. With parallelization, the MR simulation took approximately 10 hours to run and the FM simulation took about 30 hours.

There are several things to note from these results. First, one can see that there is more variability of the Young’s modulus in the MR case versus the FM case, which is to be expected. The MR case has a different network reinstated at each continuum step, while the FM case follows the deformation of the original network through the full simulation. As seen from the data in Figure 11 the elasticity moduli of the reinstated networks can vary, even though their average is close to the original network’s value. This variability is due to random elements in the reinstatement procedure such as topology of crosslinks and the number of fibers that end up attached to the walls. Unlike Figure 11, Figure 12 shows only one MR path over time for each block. Other runs with the same starting data will produce different curves, the average behavior of which will converge to the FM data. The general behavior of the evolution of the Young’s modulus of the MR and FM cases is qualitatively similar and they produce qualitatively and quantitatively similar stress fields.

5 Conclusion

This research effort has focused on the development of a novel algorithm to model heterogeneous media with time-varying microstructures. Due to computational limitations, the approach to modeling heterogeneous media has often been to ignore the inhomogeneities of the material in a purely continuum-based model. Changing mechanical properties due to changes in the material’s microstructure are not captured by such methods. Continuum-microscopic models are one possible way of incorporating microscopic information into a macroscopic model. The problem with current CM models is that the microscopic data is discarded after each continuum step and no memory of the microstructure is retained. In materials such as fibrous
Figure 12: Plots of the Young's modulus of four blocks for the FM (solid line) and MR (dashed line) cases during each continuum step.

composites, this is a problem because the microstructure changes in response to applied stresses.

The new method developed here performs the basic CM algorithm, but with the added feature that the microscopic data is saved in the form of probability distribution functions. These PDFs are then extrapolated forward in time and utilized to instantiate a microstructure at the next continuum step that resembles the microstructure of the original network at the same future point in time. This method provides an accurate way of determining the local elastic parameters (both in space and in time) that are then passed on to the continuum level equations to close the system.

The CM model presented here offers substantial computational savings over a full microscopic simulation. One goal of future work will be to reduce computational expense even further by examining ways to speed up the energy minimization procedure and also reduce the number of necessary microscopic reinstatations through sampling techniques. The method has been demonstrated for modeling a generic fibrous composite, however future work will feature applications to biological materials with the added complexity of viscous damping forces from interstitial fluids. In conclusion, this new method offers a computationally efficient algorithm for modeling continuous media that takes into account the varying mechanical properties of its heterogeneous microstructure.

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Figure 13: Plots of $\sigma_{xx}$ at three time steps for the FM (left column) and MR (right column) cases.
Figure 14: The average relative error in $\sigma_{xx}$ of a subset of blocks of the domain between the FM and MR cases during each continuum step.

References


