Continuum-Microscopic Modeling of Fibrous Materials

Jennifer Young, Rice University

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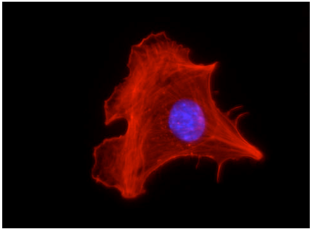
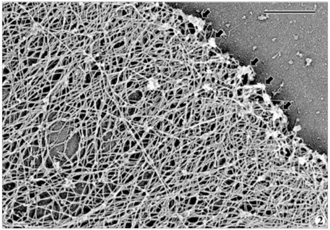
Introduction

- Original problem was to model the cytoskeleton as it undergoes deformation in the animal cell
- At the whole cell level the cytoskeleton appears to be a continuous medium (10 μm)
- Zooming in, the cytoskeleton is a complex network of crosslinked fibers (100 nm)

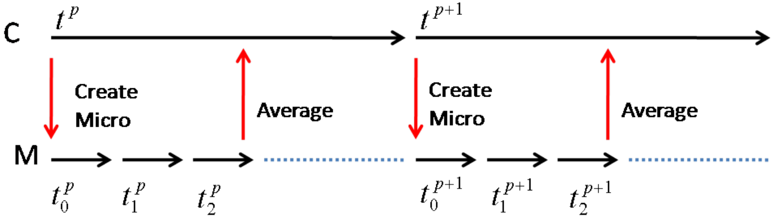




http://www.uvm.edu/ akhowe/ and http://scienceblogs.com/

A continuum-microscopic (CM) model will be a useful tool for modeling such a material

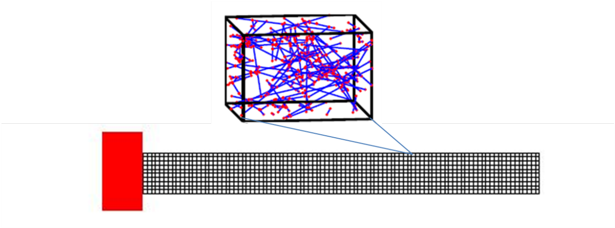
1. Create a microscopic system based on macroscopic variables
2. Run the microscopic updating scheme for a short number of time steps
3. Apply an averaging operator to get macroscopic level values from the microscopic results
4. Run the macroscopic updating scheme



Introduction

- Step 1 of the general CM method creates a new microscopic system based only on macroscopic variables
- Information from previous micro-states is lost after each continuum level step
- Goal of this research: to improve Step 1 by utilizing data from previous micro-states to assist in the reinstantiation process

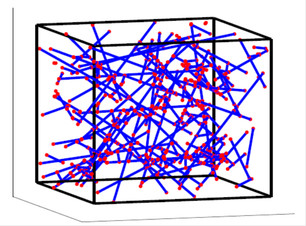
- Test case: elastic, continuous medium, whose microstructure is a complex fiber network



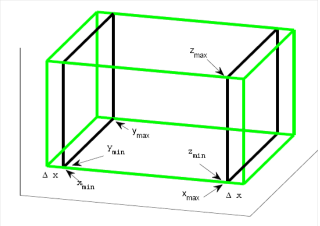
- Continuum Model: Elasticity Equations, with Hooke's Law constitutive equation
- Microscopic Model: Energy Minimization

Microscopic Model

- N, one-dimensional filaments laid in the block by choosing a starting point, length, and direction vector
- Filaments that intersect a wall are considered attached to the wall
- If the distance between two filaments is below a threshold r, then a crosslink is established



Microscopic Model



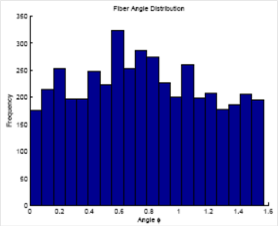
- Filaments attached to walls move with walls
- Internal filaments will be moved via an energy minimization procedure

$$E = \sum_{j=1}^{m} \left[\frac{k_j}{2} (L^j - L_0^j)^2 \right]$$

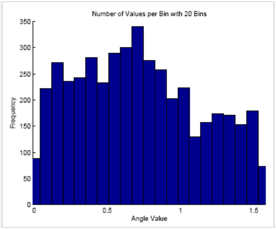
- $\nabla E = 0$ solved via an gradient search procedure

Why is a microscopic model needed at all?

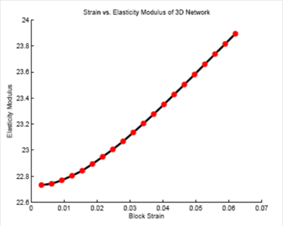
- Microstructure changes due to strain
- Mechanical parameters change due to microstructure changes



Initial Distribution



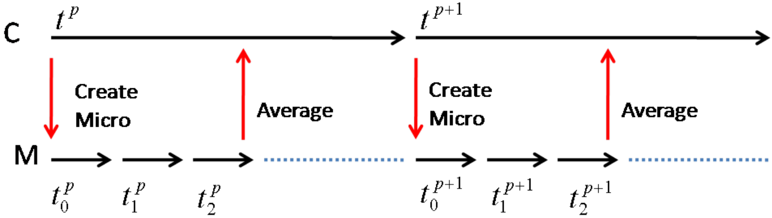
After Strain



Young's Modulus vs. Strain

Algorithm Development

- Goal: To retain information about the microstructure over time to make the recreation of the micro-system in the CM algorithm more accurate



- Data will be saved in form of probability distribution functions
- PDF estimation done with kernel estimation
- These PDFs willl be extrapolated forward in time and used to recreate the microscopic system

What data is important to save?

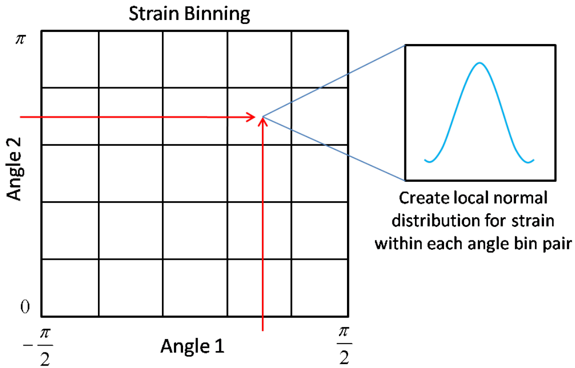
- For each filament j, its two angles of orientation θ_j, ϕ_j and its strain ϵ_j will be collected
- The variables are not statistically independent
- Ideally, a joint PDF would be best: $f(\theta, \phi, \epsilon)$
- However, joint PDF estimation and data regeneration is computationally expensive

Algorithm Development

- Replace global joint PDF with local piecewise PDFs
- Create single variable PDFs for θ and ϕ
- Divide range of angle $\theta = \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$ into M bins
- Do the same for angle $\phi = [0, \pi]$
- From the M^2 angle bin pairs, save filament strain ϵ_j into the bin corresponding to its two orientation angles
- After all strains are binned, find the mean μ and standard deviation σ^2 of the strains in each bin

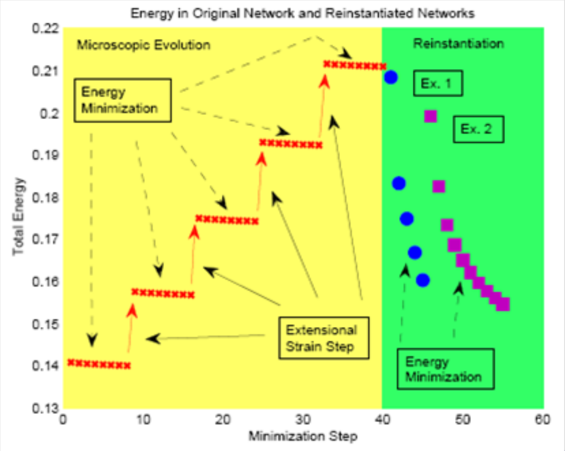
Algorithm Development

- Create a normal distribution $N(\mu, \sigma^2)$ for the strain within each bin



- During micro-system creation, assign each filament two orientation angles from $f(\theta)$, $g(\phi)$, and then assign it a strain from the corresponding $N(\mu, \sigma^2)$

Steep Drop in Stored Energy
New network = New Topology, likely not in a state of minimal energy when created

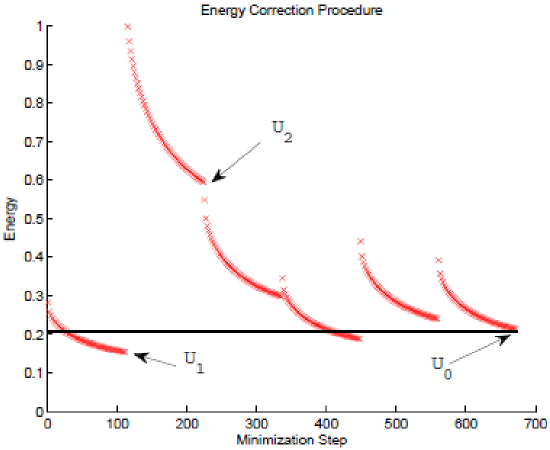


- Want the new system to have the same energy U_0 as the original system, and be in a state of minimal energy
- To achieve this, a method based on a bisection algorithm will be used
- First assign strains and angles via the strain binning method as described previously
- Run the energy minimization
- Label the new system's energy U_1
- If $U_1 < U_0$, this system and energy are marked as a lower bound

Algorithm Development

- Upper bound established by starting with the same filament configuration and strains ϵ_j but modified to a higher strain $\epsilon_j^{new} = C\epsilon_j$, with $C > 1$
- Run the energy minimization
- Label energy of this system as U_2
- If $U_2 > U_0$ then upper bound found
- If not, repeat $\epsilon_j^{new} = C\epsilon_j$ with a higher C
- Once bounds established, carry out bisection to find C that produces a system with energy minimum U_0

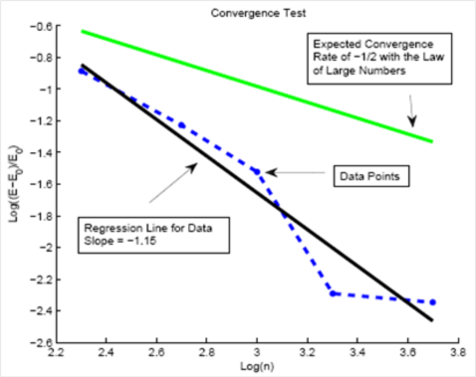
Energy Correction Algorithm



Convergence Test (no Extrapolation forward in time)

- Comparison of Young's Modulus of Original Block to average Young's Modulus of Recreated Blocks

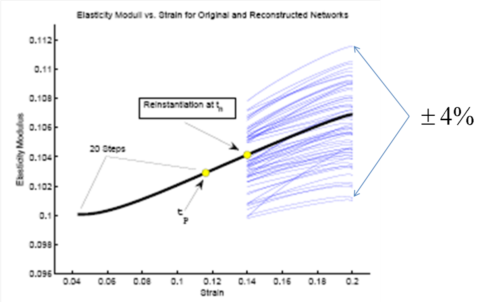
Number of Filaments	Relative Error
200	0.13
500	0.0592
1000	0.03
2000	0.00512
5000	0.0045



Algorithm Development

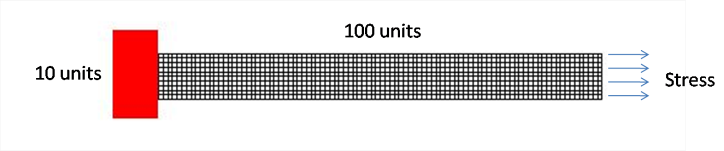
PDF Extrapolation

- After microsteps $t_0^p - t_m^p$, we will have the following PDFs $(t_0^p, \hat{f}(x, t_0^p)), (t_1^p, \hat{f}(x, t_1^p)), \ldots, (t_m^p, \hat{f}(x, t_m^p))$
- A least squares approximation is used to extrapolate a PDF for t_0^{p+1} (the start of next microscopic evolution)



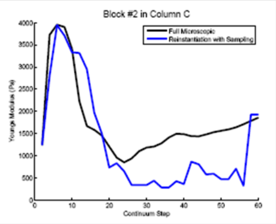
Results

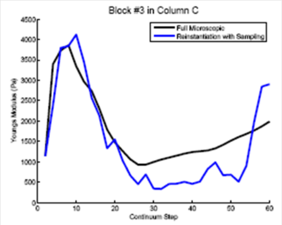
Full Simulation

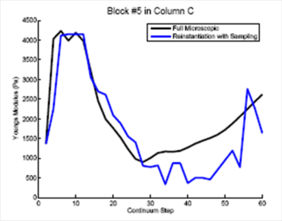


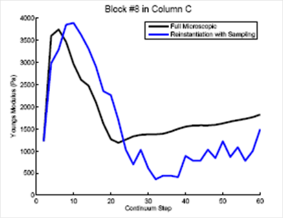
- At the macroscopic scale, the elasticity equations will be solved
- Hooke's Law: $\sigma_{ij} = C_{ijkl}\epsilon_{kl}$ is part of this system
- C_{ijkl} will be updated from the microscopic scale parameter computations

Comparison of Elasticity Moduli between a Full Microscopic Simulation and the CM Simulation



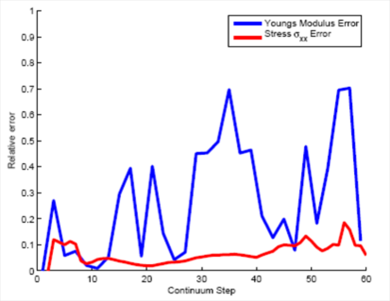






Results

Errors in Elasticity Moduli vs. Macroscopic Stress



- Errors in the macroscopic variables such as stress are small $5 - 10\%$
- Errors are a trade-off for the $50 - 75\%$ savings in computational time gained with the CM method vs. a full microscopic simulation

Summary

- Goal was to create a CM method for continuous media with space and time-varying micro-structures
- This new method utilizes micro-scale data from past time steps to recreate the micro-system at later points in time
- The algorithm was able to produce new networks with elastic parameters similar to those of the original network when this network was evolved forward to the same point in time

Reference

J. Young, S. Mitran, "A Continuum-Microscopic Model of Fibrous, Heterogeneous Media with Dynamic Microstructures", submitted to *Multiscale Modeling and Simulation* June 2010

Acknowledgments

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