Workshop « Soft Material Models »

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Three-dimensional hyperelastic model based on a micromechanical approach for rubber-like materials

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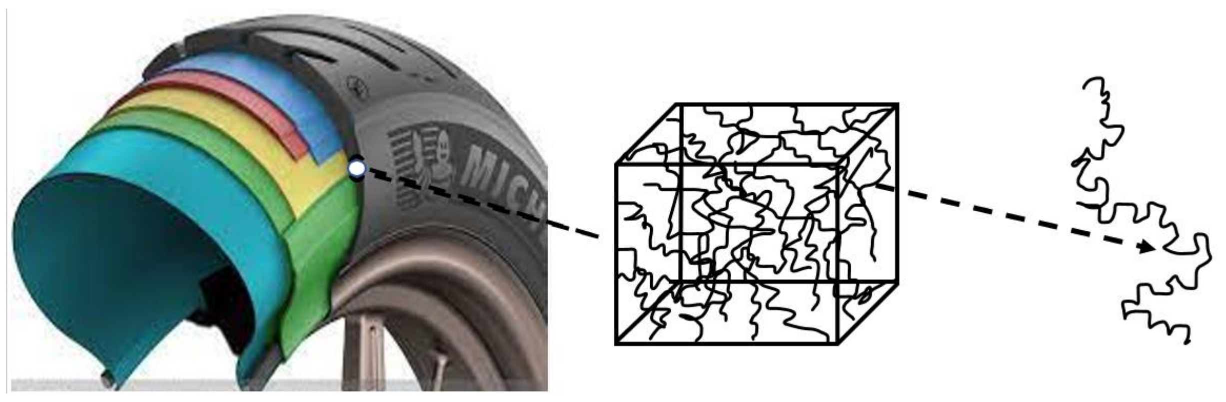
Abstract

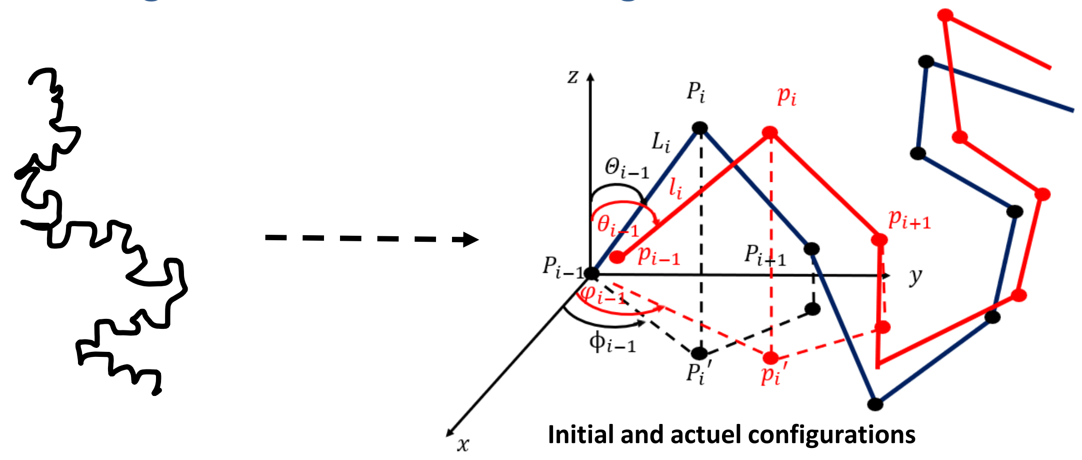
In this work, we propose a three-dimensional hyperelastic model to describe the behavior of rubber-like materials. At the scale of the Representative Volume Element (RVE), we assume that, for each macromolucular chain, the segments of the chains are deformable and that there is a bending and torsion energy between two consecutive segments. We propose to model each macromolecular chain using micro-mechanical elements: elastic bars to represent the segments between cross-linking points and elastic spire to illustrate the flexibiliy of rotations arround the cross-linking points.

Modelisation

❖ **From the structure to the macro-chain: multiscale representation**



❖ **A single chain macromolecular: geomitrical modelisation**



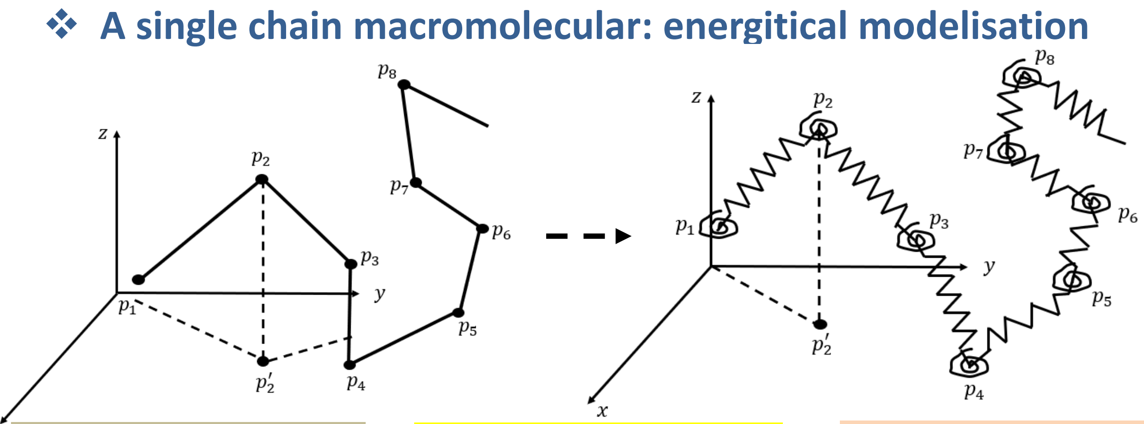
Initial and actuel configurations

Deformation variable: $\Delta l_i = l_i - L_i$ $\quad \Delta\varphi_i = (\varphi_i - \varphi_{i-1}) - (\phi_i - \phi_{i-1})$

$\Delta\theta_i = (\theta_i - \theta_{i-1}) - (\Theta_i - \Theta_{i-1})$

$\dfrac{r - r_0}{r_0}$ $\quad r_0, r$: The end to end distance (initial and actuel)

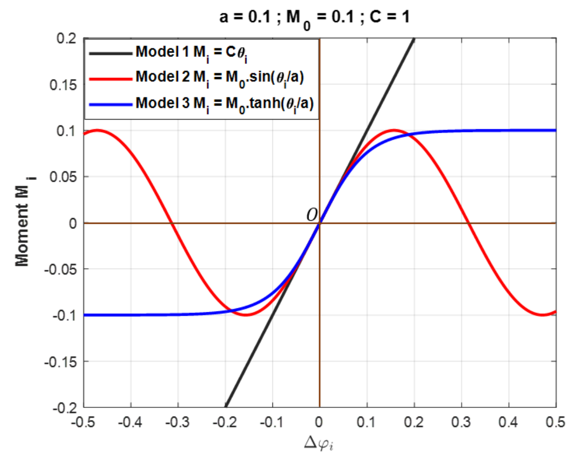
❖ **A single chain macromolecular: energitical modelisation**

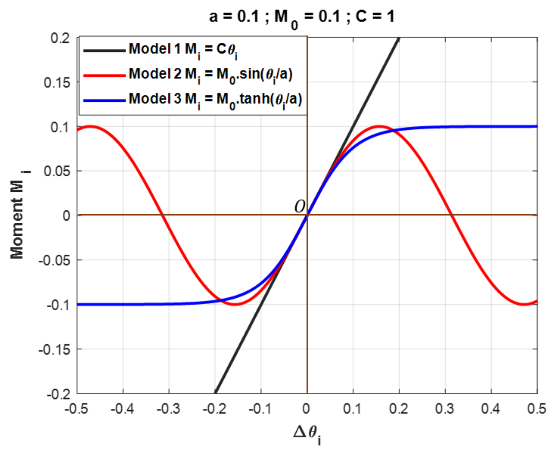


Tensil $w_{t_i}(\Delta l_i)$ + bending $w_{\varphi_i}(\Delta\varphi_i)$ + torsion $w_{\theta_i}(\Delta\theta_i)$

For the tensil energy we choose: $w_{t_i}(\Delta l_i) = \frac{1}{2} K\,(\Delta l_i)^2$

For the bending and torsion energy we have:



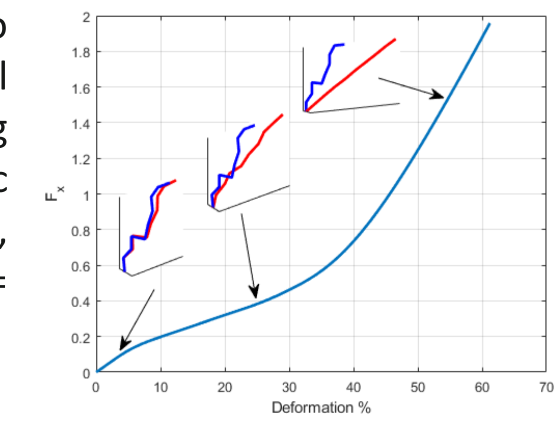


$w_{\varphi_i}(\Delta\varphi_i) = a.M_0.\ln\left(\cosh\left(\frac{\Delta\varphi_i}{a}\right)\right)$ $\quad w_{\theta_i}(\Delta\theta_i) = a.M_0.\ln\left(\cosh\left(\frac{\Delta\theta_i}{a}\right)\right)$

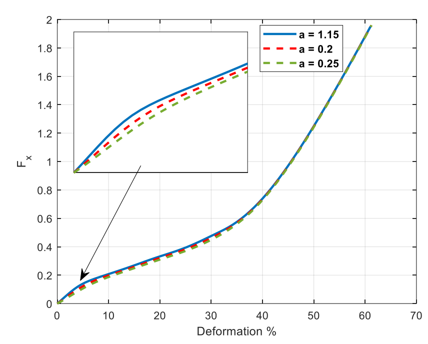
Results

❖ **Numerical application: A single chain formed by 9 effective segments**

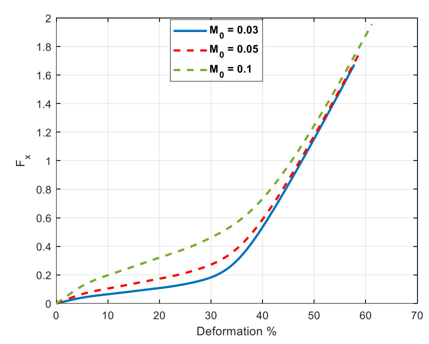
This modeling allows to find the classical response curves using only three characteristic parameters $a = 0{,}2\text{rad}$, $M_0 = 0{,}1\text{N.nm}$ and $K = 10\text{N/nm}$.



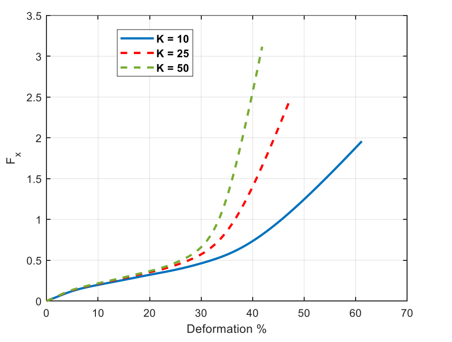
Effect of the 3 characteristics of the material a, M_0, K, on the behavior of the polymer



Influence of a for $M_0 = 0.1\text{N.m.}$ and $K = 10\text{N/nm}$.



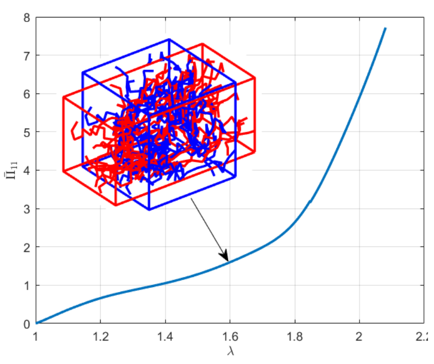
Influence of M_0 for $a = 0.2\text{rad}$ and $K = 10\text{N/nm}$.



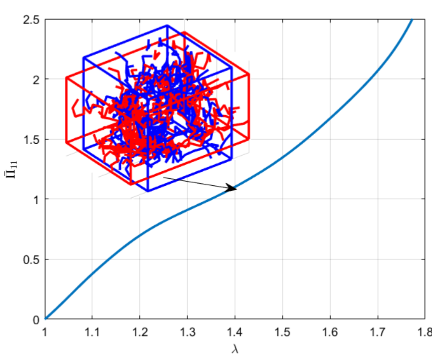
Influence of K for $a = 0.2\text{rad}$ and $M_0 = 0.1\text{N.m.}$

We can thus see that: a controls the first disentanglement zone, M_0 controls the second unfolding zone, K controls the third crystallization zone under large deformation.

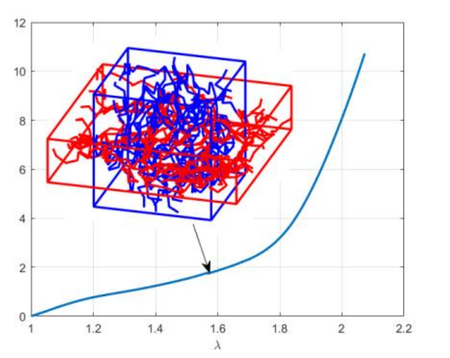
❖ **Numerical application: Representative Volume Element (RVE)**



Uniaxial tension $\mathbb{F} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 1/\sqrt{\lambda} & 0 \\ 0 & 0 & 1/\sqrt{\lambda} \end{bmatrix}$



Pure shear $\mathbb{F} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1/\lambda \end{bmatrix}$



Equibiaxial tension $\mathbb{F} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & 1/\lambda^2 \end{bmatrix}$

Response curves of RVE formed by 25 chains $\overline{\Pi}_{11}$ component of the 1st Piola-Kirchhoff stress tensor as a function of $F_{11} = \lambda$, for three boundary conditions: uniaxial tension, pure shear and equibiaxial tension. The parameters material used are $a = 0{,}1rad$ for $M_0 = 10^{-8}\text{N.m.}$ and $K = 10^{-8}\text{N/nm}$.

Conclusion and perspectives

In this work, we have proposed a three-dimensional hyperelastic model based on micro-mechanical elements for rubber-like materials. Numerical simulations have been presented, using this model, in the case of a single macromolecular chain and in the case of a 3D Representative Volume Element (RVE) formed by several macromolecules distributed in a random way. In terms of perspectives, we plan to enrich this approach by introducing irreversible micro-mechanisms by Mullins effect.

References

[1] Ouardi, A. & Boukamel, A. & Damil, N. (2022). Towards a macro-chain polymer model using a micromechanical approach; ECCMR 2022, Politecnico di Milano, Italy, 07-09 September.