New coarse grained approach to study polymer networks

Rencontres Des Jeunes Physicien.ne.s 2021

Gérald Munoz March 18, 2021

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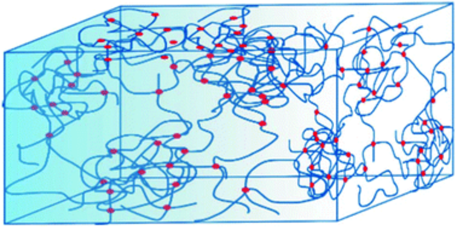
Polymer network



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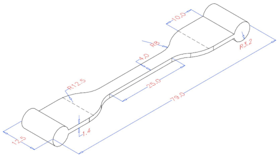
Gérald Munoz, Alain Dequidt, Nicolas Martzel, Ronald Blaak, Étienne Munch, Patrice Malfreyt

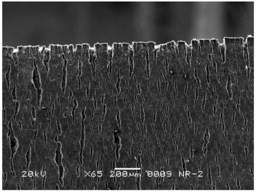
Framework and Project

- Multiscale modeling for polymer materials
  - Molecular dynamics (atomistic)
  - Dissipative Particle Dynamics (coarse-grained)
  - Elastic Network Model (ENM, topological constraints)
- Thesis project
  - What is the link between heterogeneity of the microstructure and mechanical properties until rupture ?
  - Modeling crosslinked polymer by using an ENM

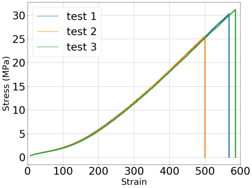
Experimental studies



H3 tensile specimens



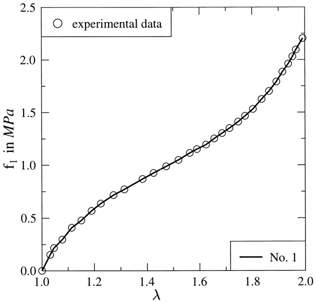
SEM micrographs



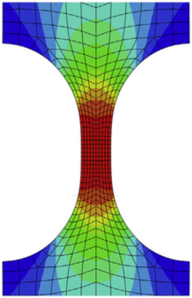
Uniaxial stress–strain behavior

- Stress-strain behavior not well understood
- Can it be explained by heterogeneity ?

Traditional theoretical study



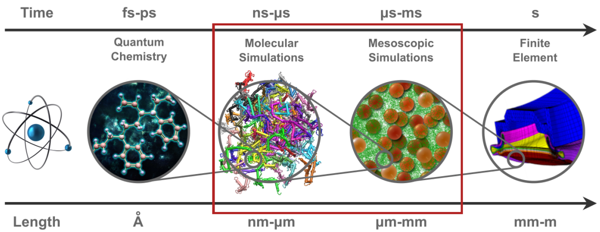
Extended tube model



H3 finite element calculation

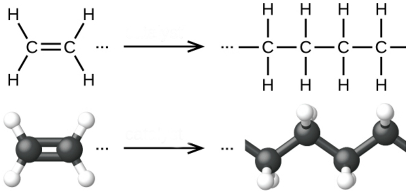
- Phenomenological law
- Fitting physical parameters (chain length, Kuhn length, entanglement mass...)

Multiscale modeling for polymer materials

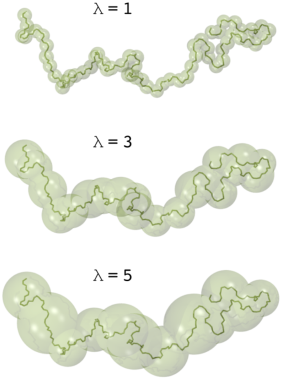


- Develop methods for the mesoscopic scale (topological constraints: crosslink, entanglement)
- Using polymer properties as input (chain length distribution, entanglement mass, ...)

Modeling elastomers: coarsegraining procedure

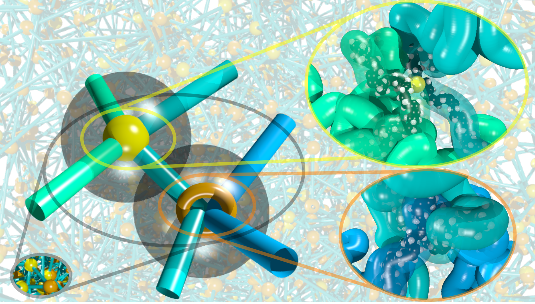


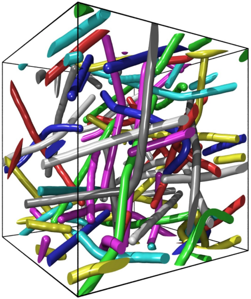
Atomistic scale



Coarse grained model

Elastic Network Model

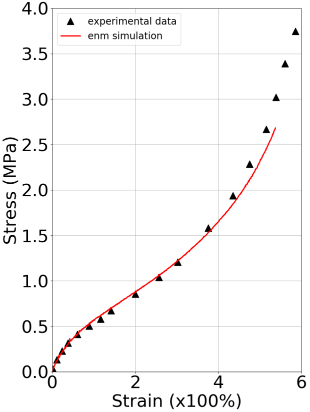


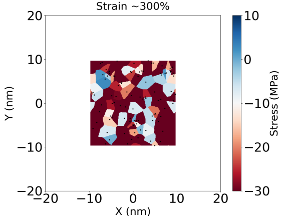


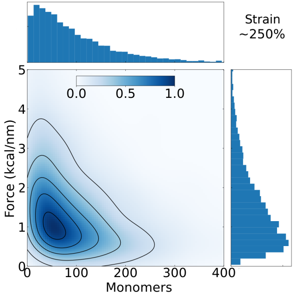
- Each link is characterised by its own specific monomer number
- Chain forces act along the end-to-end vector
- What is the link between heterogeneity of the microstructure and mechanical properties ?

Stress distribution analysis

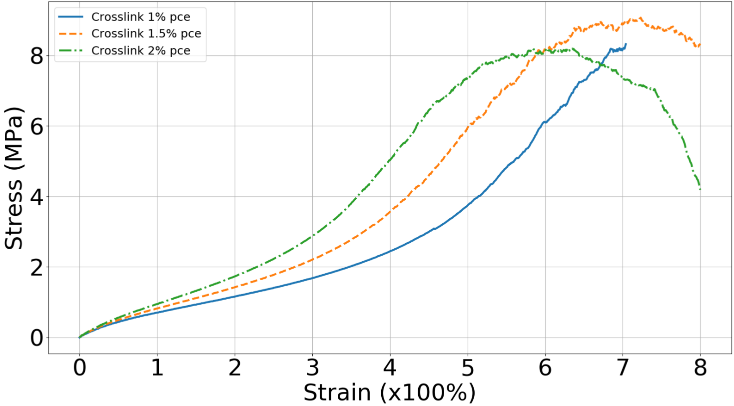
local and global stress heterogeneity







Introduction of rupture criteria



- In agreement with experiments
- Breaking mechanism : maximum chain force

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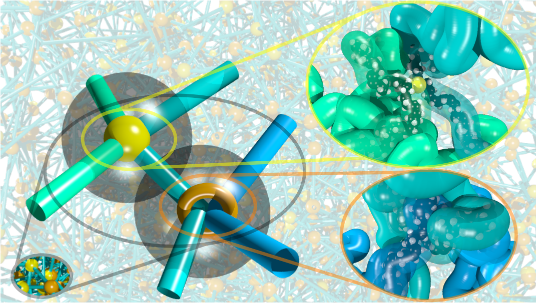
Conclusion



- Simulate deformation until rupture
- Understand microstructure and topological effects
- Study others systems of interests

New coarse grained approach to study polymer networks

Thank You !

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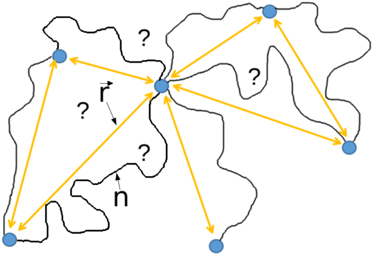
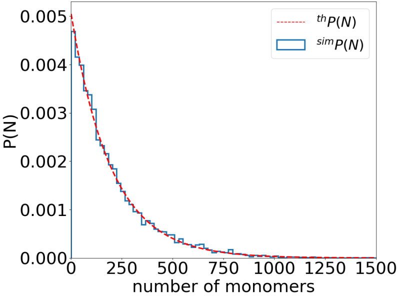
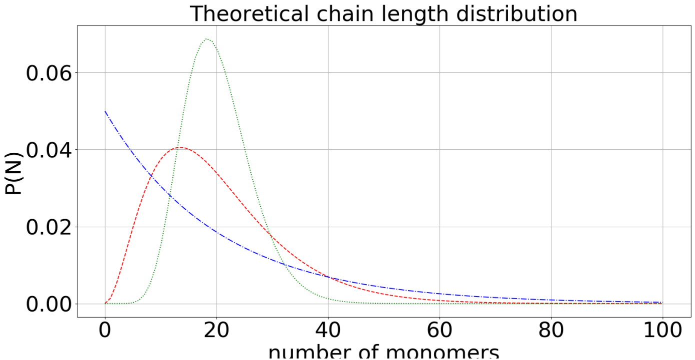
Network generation

$$P(n, \vec{r}\,) = P(n) \times P(\vec{r}\,|n)$$

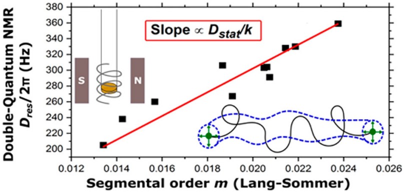




Chain length distribution



Network generation: Coupling Experiment - Theory



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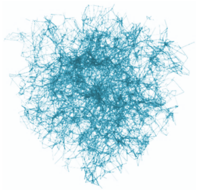
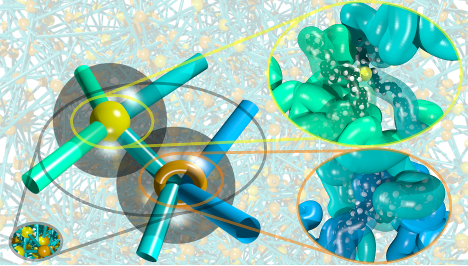
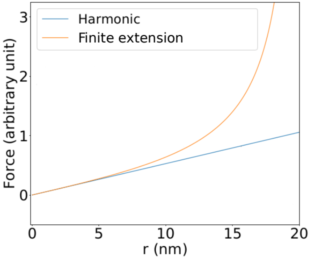


- $P(n, \vec{r}\,) = P^{\mathrm{exp}}(n) \times P^{\mathrm{th}}(\vec{r}\,|n)$
- Comparison of experimental and model results

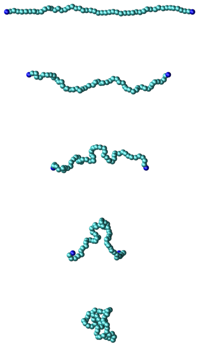
Force field

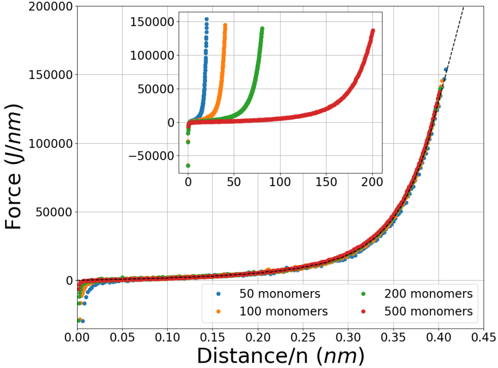




- Chain forces act along the end-to-end vector
- Each link is characterised by its own specific chain length (nb)

Force field: Theory vs Coarse grained





- Extract a master curve and produce a coarse grained attractive potential