ESR11: Modeling the nonlinear rheology of reversible double dynamics networks

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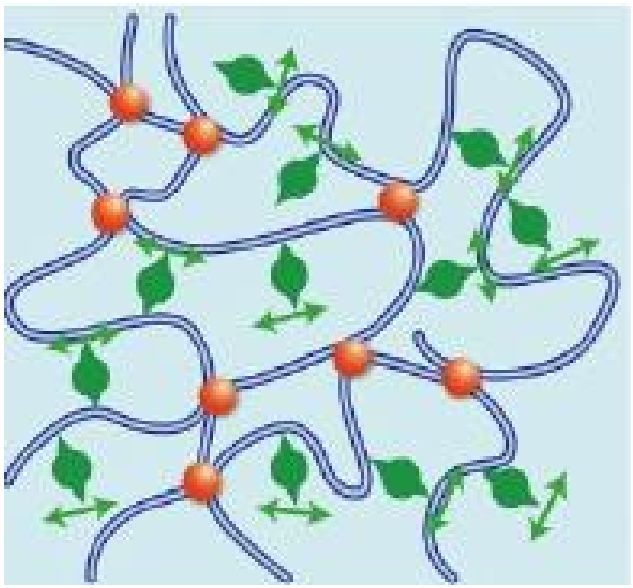
INITIAL TRAINING NETWORK
DCDnet

Background

- Ph.D., Sep. 2018-Current, Department of Chemical, Materials, and Production Engineering, University of Naples Federico II, Italy
- M.S., Sep. 2015-Jun. 2018, School of Civil Engineering & Transportation, South China University of Technology, China
- B.S., Sep. 2011-Jun. 2015, School of Civil & Hydraulic Engineering, Hefei University of Technology, China

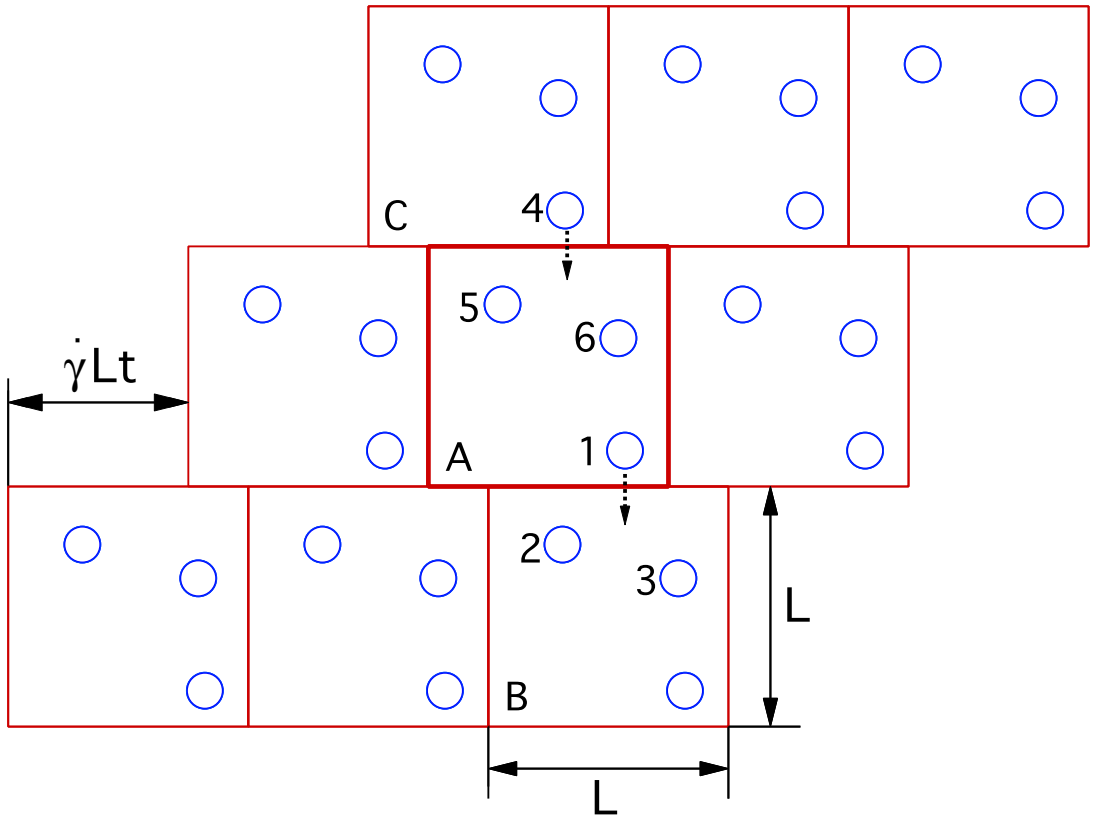
Research: goals

- We are aiming at simulating the nonlinear viscoelastic properties of a sort of associating polymers. Scuh associating polymers have two kinds of stickers along the backbone, one is reversible and the other one is somewhat permanent, and can form transient networks.



Research: methodology used

- To simulate the movement of molecules, we resort to Browninan dynamics simulations. Besides, periodic boundary conditions are used when we have interacting molecules (polymer network, for example).



Research: results

- Up to now, we have established the program for the 2-D transient networks. By plotting the conformations of the molecules and comparing with the analytical solutions, we can say that our program is valid.

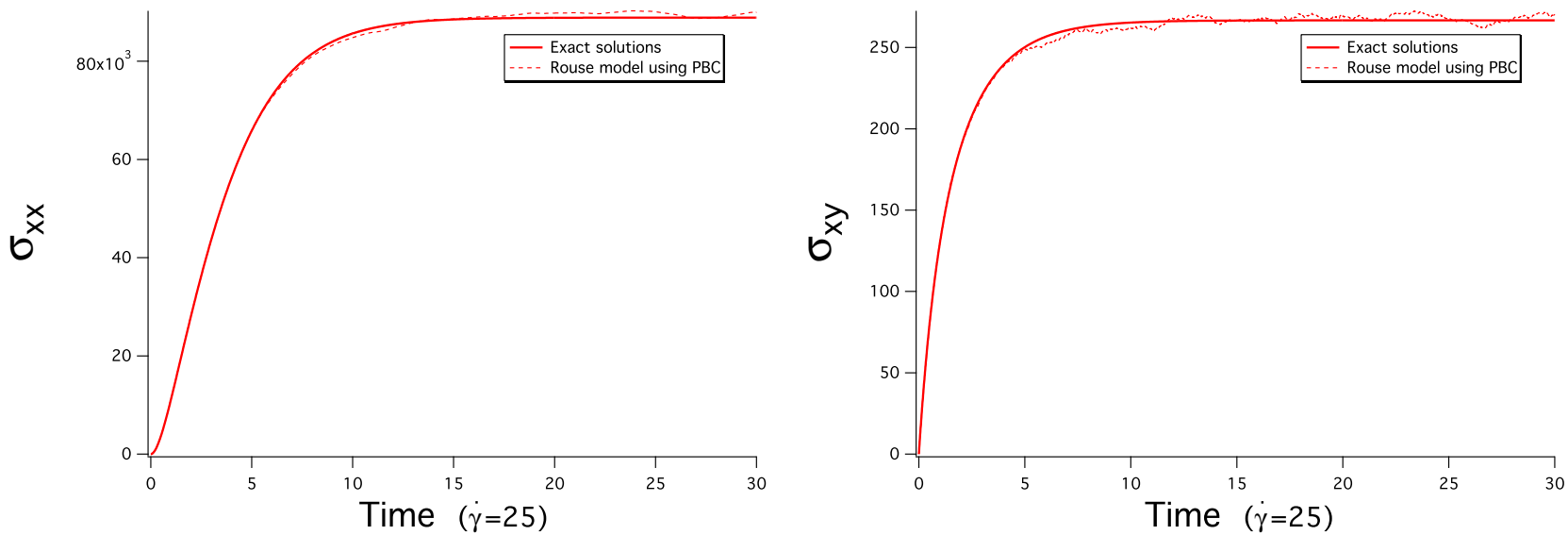


Figure 1: Stress tensor (molecules:10000, beads for every molecule:5).

Training and Scientific Activities

- Training
  - Advanced Thermodynamics and Advanced Transport Phenomena (prof. Giovanni Ianniruberto)
  - Biomechanics
  - Summer School on smart nanomaterials for drug delivery (prof.ssa Veronica Ambrogi)
- Scientific activities
  - DTU – O. Hassager (M20-M23): perform specific extensional measurements in order to address questions from modeling.
  - Industrial secondment: tesa (M43-M44) – understand the role of chain stretching and strain hardening on the resistance of the DDNs.

Plans for the future

- Plan A
  - Three years later, hopefully, find a post-doc position funded by MSCA.
  - Five years later, to be a lecturer in the university.
- Plan B
  - Three years later, enter the industry.
  - Five years later, to be a lecturer in the university.