Data-driven network models for the coupled nonlinear response of soft electroactive nanomaterials

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Background

Soft matter systems such as gels and polymer networks possess a range of interesting and technologically useful properties: they have been the focus of intense scientific research, leading to entire industries being built around their development and utilization. The potential of these technologies is far from being spent - dielectric elastomers, to provide but one example, promise great advances in industries as diverse as soft robotics [1], biotechnology [2] and power engineering [3]. However, current technologies do not have sufficient material properties to bring any of these advancements to fruition. The enhancement of the mechanical and thermodynamic properties of various soft matter systems is naturally a question of great practical interest.
One approach to the development of soft materials with enhanced properties is via the inclusion of nanoparticles in the manufacturing process.

This project is based around the modelling and simulation of soft materials, with added nanoparticles, that exhibit electromechanical responses. Such materials are excellent examples of complex systems, as

- the responses are typically highly non-linear, with the electrodynamics and the mechanics of the systems are inherently coupled.
- the system incorporates multiple distinct, yet interacting components.
- the macroscopic response is heavily dependant on the microstructural features of the system.

As with most complex systems, traditional modelling methods are either inefficient or insufficient: polymer networks, for one, are enormous and due to significant variations possible in microstructural details, a very large number of molecular dynamics simulations must be performed in order to gain even a decent ensemble average. To this end, a large part of the project will be based around the application of Bayesian inference on a coarse-grained polymer systems, specifically through Gaussian process regression: the aim is the generation of efficient surrogate models that provide a means to work with systems that are otherwise near-intractable.

Project aims

The main goal of this project is the development of surrogate models that model complex electroactive polymer behaviour. This will require the following components:

- A medium for the virtual design of soft nanocomposites at the microstructural level, via a coarse-grained representation.
- A means for the evolution and simulation of multiple realisations of the design.
- A method for the conversion of the generated data to build a network model via Gaussian process regression for the prediction of important mechanical and thermodynamic quantities.

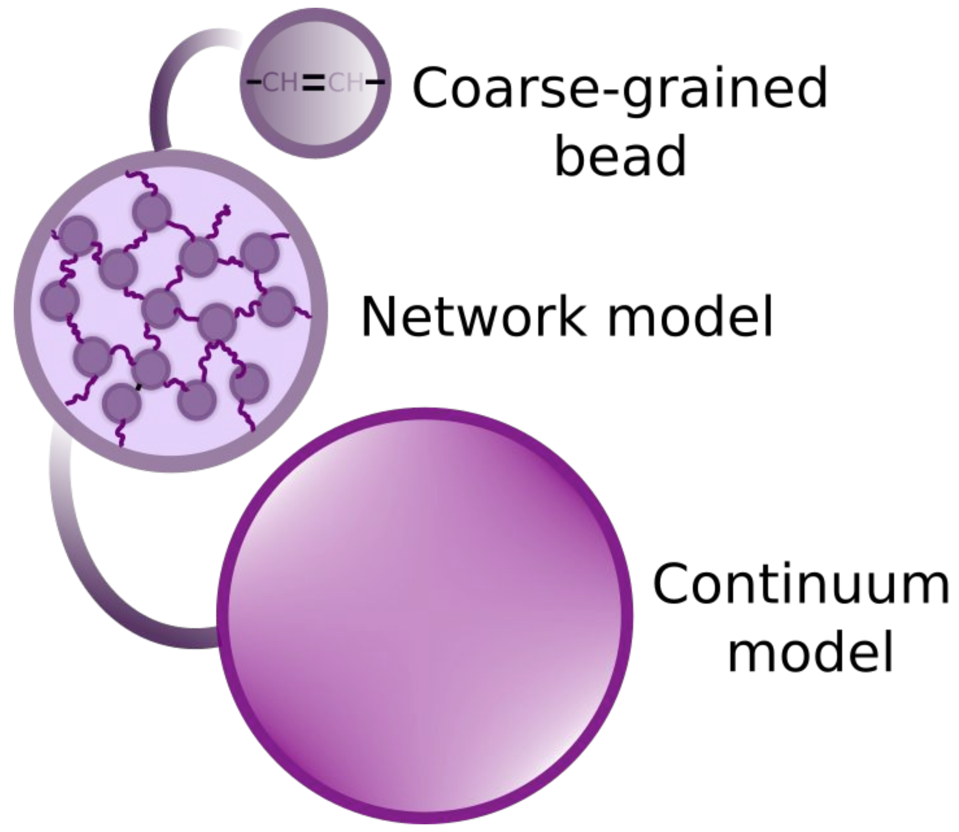

Figure 1: Schematic of the scales that are to be covered by the software

Essentially, the software will be an integrated tool for the prediction of macroscale properties of materials from the microstructure. The basic goal of this project is the prediction of the strain energy density function, also known as the unit Helmholtz free energy, for a dielectric polymer nanocomposite. Once this result is achieved, the project can go in any or all of the following directions:

- Incorporating finite element analysis to extend the software to a truly multiscale methodology.
- Further development on the microscale by considering and implementing novel coarse-graining methodologies [5].
- Adding to the variety of materials that may be simulated, i.e nanocomposite hydrogels, colloidal nanocomposites, etc.

Generation of polymer networks

Naturally, the most important goal here is the development of the software, which is currently dubbed *nanoPoly*. Figures 1, 2 and 3 demonstrate the generation of a series of polymer conformations, with interchain features such as crosslinking incorporated. The software has been developed with complete freedom of design for the user in mind: as such nearly everything about the chains is completely customisable.

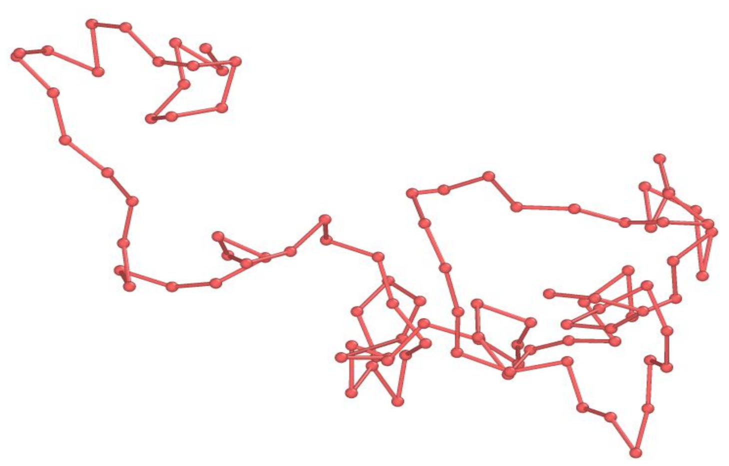
Figure 2: A simple homopolymer chain with 100 beads, generated with nanoPoly.

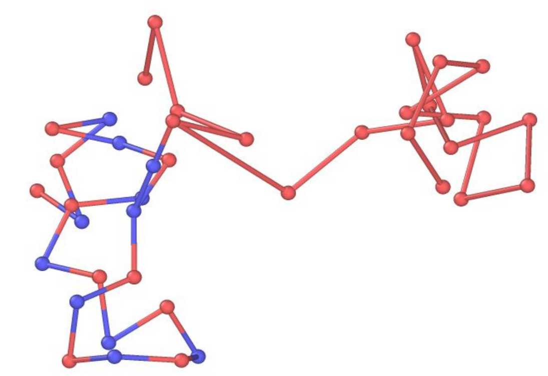
Figure 3: A demonstration of the crosslinking feature available with nanoPoly, linking a homopolymer with a copolymer.

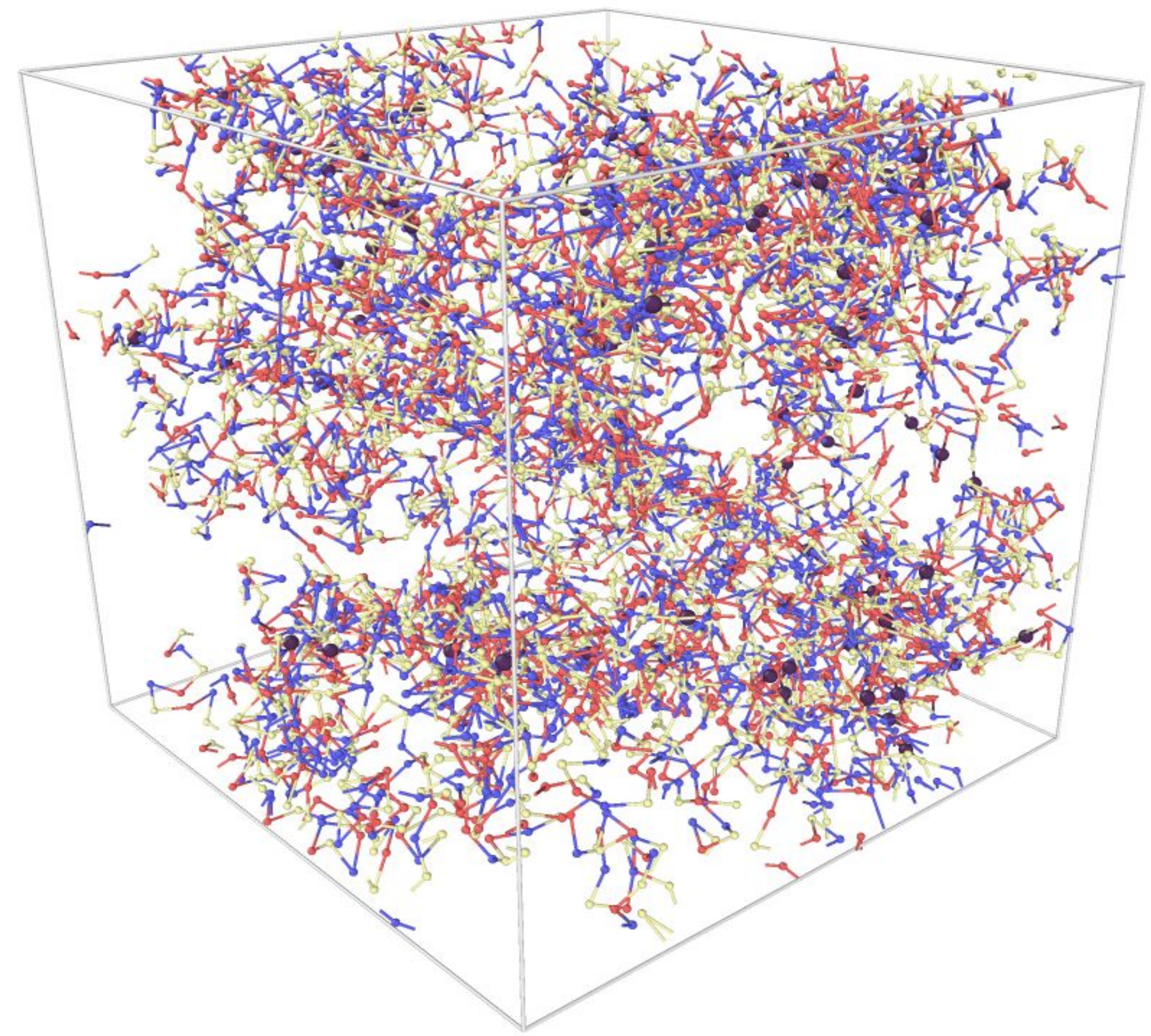
Figure 4: A complex network system composed of five chains, each built from 1000 beads, generated with nanoPoly. The chains are composed of three different beads with different properties. The dark purple beads denote crosslinkers, of which there are a hundred.

Current goals

The short term goals for the software, to be completed by summer, are the following:

- Implement molecular dynamics simulation capabilities for the software.
- Generate data on the stress-strain curves of various systems with a different number of crosslinks.
- Via Gaussian Process regression, build a non-parametric model that predicts the stress-strain curves of the network for different values of the crosslink density.

Effectively, the aim is to build a working version of *nanoPoly*. The capabilities of this software will then be improved to handle complex electroactive soft matter systems.

Citations:

[1] Dielectric Elastomer Actuator for Soft Robotics: Applications and Challenges
Youn et. al. in *Applied Sciences*, Jan 2020
[2] Theory of Dielectric Elastomers
Suo in *Acta Mechanica Solida Sinica*, Dec 2010
[3] Modelling and testing of a wave energy converter based on dielectric elastomer generators
Moretti et. al in *Proceedings of the Royal Society A*, Feb 2019
[4] Energy renormalization for coarse-graining polymers having different segmental structures
Xia et. al. in *Science Advances*, Apr 2019