PhD Project Proposal 5

Title: Optimising Magneto-Polymer Gels by Combining Molecular Simulations and Machine Learning

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Magneto-polymer gels are smart materials composed of polymeric hydrogels or networks with embedded magnetic particles whose structural, mechanical and rheological properties can be reversibly and efficiently controlled by applying external magnetic field. The biocompatible, superelastic and stimuli-responsive features of these materials lead to wide technological and biomedical application potential, such as in elastomers, artificial biological tissues, drug delivery, cell adhesion, proliferation and differentiation. However, magneto-polymer gels constitute complex systems with different emergent behaviour. Since these systems are governed by many control variables, finding conditions that optimise certain properties are very challenging.

To tackle this problem, we want to employ a fairly detailed molecular model where inter-connected beadspring chains represent the polymer network forming the gel to which we add a collection of magnetic particles. [1,2] Particles attract and repel each other via steric, electrostatic and magnetic interactions. The dynamics of this interacting and highly non-linear system will be studied numerically for a selection of model parameters by Molecular Dynamics simulations, which integrate the equations of both translational and rotational motions of all particles where friction and Brownian effects of unresolved solvent molecules are incorporated implicitly. With the trajectories of all particles at hand, we can analyse the numerical results to determine all relevant information. In particular, we will study the long- and short-time diffusion behaviour, as well as internal structures and stresses which are relevant for the mechanical properties of the system.

Since the number of model parameters is large and the molecular simulations are time-consuming, these “computer experiments” can explore only a very limited region in parameter space. Guessing optimal parameters from such limited information is unsatisfactory. Therefore, we use the data obtained from molecular simulations as training and test data for supervised machine learning algorithms. [3] Our previous studies have shown that neural networks with random forest and extreme gradient boosting algorithms are able to learn such data sets very well [4]. Once the network has successfully been trained, we are able to reliably predict the model behaviour for parameter values that we have not simulated. This then allows us to explore the parameter space more fully and therefore find parameter values that optimise our target functions. We will then test these predictions by simulating the molecular model for the predicted optimal parameter values to see whether our target properties are indeed correctly predicted. In case the prediction is not accurate, we will perform additional molecular simulations to enhance the training set and re-run the training and test steps of the machine learning algorithm.

The project is structured along with the following successive tasks:

A. *Year1:* Literature review of and study of molecular dynamics [1,2], polymer networks and machine learning algorithms such as feature engineering and neural networks [3].

B. *Year 2:* Molecular simulations and data analysis using feature engineering and unsupervised learning approaches to identify and characterise the physical properties of the involved variables.

C. *Year 3:* Formulation of *data cube* on molecular simulations and polymer network properties and design of deep neural networks for creating a cost-effective alternative to expensive simulations.

Student profile: Bachelor 2:1 or Master in Mathematics, Statistics or Computer Science.

References:

1. Ilg, P., Stimuli-responsive hydrogels cross-linked by magnetic nanoparticles, Soft Matter, 2013, 9, 3465.
2. Wang, Z. W., Holm C., Müller, H. W., Molecular dynamics study on the equilibrium magnetization properties and structure of ferrofluids, Physical Review E, 2002, 66, 021405.
3. Ojha, V. K., Schiano, S., Wu, C. Y., Snášel, V., & Abraham, A Predictive modelling of die filling of the pharmaceutical granules using the flexible neural tree. Neural Computing and Applications, 2018, 29, 467-481.
4. Desai SV, The study of diffusion of nano-particles in polymer and ferrofluids using machine learning, 2021, University of Reading, Master Dissertation.