IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Modelling dynamics and flow for soft fibre systems**	
Project Number	**IMURA0889**	
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Research Clusters:

Highlight which of the Academy's CLUSTERS this project will address?
*(Please nominate JUST **one.** For more information, see www.iitbmonash.org)*

1	*Material Science/Engineering (including Nano, Metallurgy)*
2	*Energy, Green Chem, Chemistry, Catalysis, Reaction Eng*
3	*Math, CFD, Modelling, Manufacturing*
4	*CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control*
5	*Earth Sciences and Civil Engineering (Geo, Water, Climate)*
6	*Bio, Stem Cells, Bio Chem, Pharma, Food*
7	*Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng*
8	*HSS, Design, Management*

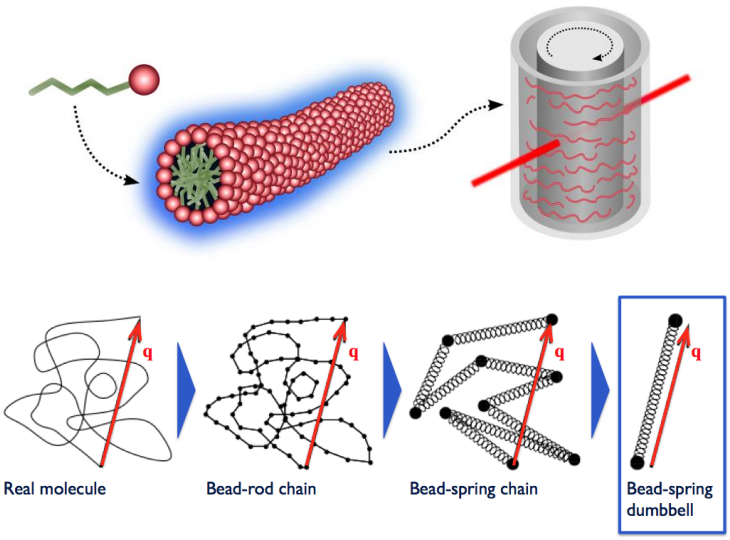
Research Themes:

Highlight which of the Academy's Theme(s) this project will address?
(Feel free to nominate more than one. For more information, see www.iitbmonash.org)

1	*Advanced computational engineering, simulation and manufacture*
2	*Infrastructure Engineering*
3	*Clean Energy*
4	*Water*
5	*Nanotechnology*
6	*Biotechnology and Stem Cell Research*
7	*Humanities and social sciences*
8	Design

The research problem

The flow and texture of soft and self-assembled systems is implicated in phenomena as diverse as shampoo formulation and the functioning of proteins in biological cell membranes. Crucially, the ability to link nano- and micro-structure to bulk properties is an outstanding issue. Although we can make high resolution measurements of such systems at small and large length-scales, from electron microscopy (nanometre resolution) to rheology (bulk scale flow dynamics), concepts linking the two require new modelling insight. We are particularly interested in soft systems, and especially those that self-assemble, such as wormlike micelles, self-assembling proteins and biological fibers, non-covalent polymers, and hydrogels. By understanding how flexibility and connectivity in these systems manifest in bulk properties such as non-Newtonian flow behaviour, we can better understand the physical world, and better design new formulations to save energy and resources.



A major outstanding challenge in the field of complex fluid dynamics is in linking directly the structural features of the fluid (for example, for flexible chains with finite volume, the overall contour length, persistence length over which the chain is locally rigid, total volume fraction and interaction potential between chains) with the bulk properties of the fluid. Difficulties arise as these systems cannot be analytically “solved” like hard sphere analogues, due to the complexity of their geometry. Coupled to this, real systems show considerable nonidealities such as chain branching, looping, entanglement, etc. Developing a model that can systematically link measured structural features such as these to how these materials flow and deform will be a huge step forward for the field.

In the case of solutions of linear polymer molecules, many static and dynamic properties, and in particular rheological properties, have been shown to be a consequence of the large scale and long-time behaviour of polymer molecules. As a result, significant progress in the description of the flow behaviour of solutions of linear polymer molecules has been made with the help of coarse-grained models such as bead-spring chains, which ignore details at the level of chemistry, but are still able to capture the essential features of their behaviour. Computational approaches based on such models are referred to as mesoscopic simulations.

Mesoscopic simulations of polymer solutions have enabled the relation between physical phenomena occurring on a molecular scale with flow behaviour on a macroscopic scale to be clearly understood. Mesoscopic simulations have not yet been applied to studying the rheological behaviour of solutions of wormlike micelles. The similarity of the properties of wormlike micelles and polymer molecules suggests that successful approaches in the latter case could be fruitfully applied to the former. The central aim of the current project is to develop a simulation framework within which wormlike micellar solutions can be studied with coarse-grained models.

References:

Kailasham, R., Chakrabarti, R., & Prakash, J. R. (2018). Rheological consequences of wet and dry friction in a dumbbell model with hydrodynamic interactions and internal viscosity. *J. Chem. Phys*. 149(9), 094903.

Moore, J. E., McCoy, T. M., Sokolova, A. V., de Campo, L., Pearson, G. R., Wilkinson, B. L., & Tabor, R. F. (2019). Worm-like micelles and vesicles formed by alkyl-oligo (ethylene glycol)-glycoside carbohydrate surfactants: The effect of precisely tuned amphiphilicity on aggregate packing. J. Colloid Interface Sci. 547, 275-290.

Project aims

The primary aim of this project is to construct a model that can predict the bulk flow properties of biological and synthetic complex fluids, particularly those comprising wormlike chains or soft fibres.

This will involve extending the current multi-particle mesoscopic simulation algorithm developed in the molecular rheology group for describing linear polymer chains to wormlike micellar solutions, with a view to numerically calculating static, dynamic and rheological properties. Mesoscale hydrodynamic simulation approaches are essential, because only they allow one to reach the large length and time scales which are required to capture the long structural relaxation times in flow. Most importantly such simulations include thermal fluctuations and hydrodynamic interactions, which are indispensable for a proper description of wormlike micellar solution dynamics. Essentially, wormlike micelles can be modelled as a solution of coarse-grained chain molecules that have been formed spontaneously from simple dumbbells models attached to each other at their ends by reversible bonds. The dumbbells represent the persistence length of the wormlike micelle. The new multi-particle algorithm, which will be unique in the world, will give an unprecedented opportunity to examine the influence of (i) the instantaneous wormlike micelle length, (ii) the strength of the attraction between dumbbells, (iii) the concentration and polydispersity of the wormlike chains, and (iv) the flow strength, systematically. The creation and destruction of transient wormlike micelles in flow can be directly visualised, and their relation to the development of macroscopic stress in the solution can be explored.

The simulations will be informed by nanostructure measurements from scattering and microscopy, and results of simulations will be used to model and predict rheological behaviour of the systems in different flow geometries. The systems of study will begin with simple model fluids in the form of viscoelastic dispersions of wormlike chains, relevant to personal care products and drilling fluids. Additional complexity will then be added in the form of branched, entangled and gelled systems with higher order structures.

Expected outcomes

> A model that can accurately describe the flow dynamics and rheology of soft chain dispersions, based on nanostructural inputs from real measurements.

> Comparison of the model to obtained experimental rheology and flow birefringence data, demonstrating its effectiveness and applicability.

> Prediction of phase and flow behaviour for new systems, allowing iterative development and testing of new compositions.

These outcomes will result in high quality journal publications within the fields of fluid dynamics and soft systems, with exemplar outputs demonstrated in recent publications from the participating academics. In addition, we anticipate that code or methods as applied to industrially relevant systems such as wormlike micelles in personal care may be protected by patent; Tabor has recent experience in this area for similar work, with submission of a recent patent for wormlike micellar fluids (WO2019/136517).

How will the project address the Goals of the above Themes?

This project will make fundamental contributions to nanotechnology (industrial fluid formulation/flow dynamics) and biotechnology (rheology and flow of biologically relevant fibres and soft systems). This will be achieved by using computational methods to “close the gap” in understanding how the fundamental physical structure of such systems results in their unusual (and broadly unpredictable or unexpected) bulk physical properties, such as viscoelasticity.

Capabilities and Degrees Required

The following capabilities are essential:
1. Excellent training in mathematics and numerical methods (biology knowledge is not mandatory)
2. Proven experience with computer programming in high level languages
3. Ability to write and communicate fluently
4. Strong background in Engineering/Physics (Either M Sc in Physics or B Tech/BE in Mechanical/Chemical/Electrical Engg)

While the topic has a biological context, students without a background in physics or engineering will not be considered.

Potential Collaborators

Please visit the IITB website www.iitb.ac.in OR Monash Website www.monash.edu to highlight some potential collaborators that would be best suited for the area of research you are intending to float.

Select up to **(4)** keywords from the Academy's approved keyword list **(available at http://www.iitbmonash.org/becoming-a-research-supervisor/)** relating to this project to make it easier for the students to apply.

Computational Fluid Dynamics and Mechanics, BioScience, Modelling and Simulation, Smart manufacturing