IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Influence of Wet and Dry Friction on Polymer Dynamics**	
Project Number	**IMURA0899**	
Monash Main Supervisor (Name, Email, Phone)	Ravi Jagadeeshan, ravi.jagadeeshan@monash.edu	*Full name, Email*
Monash Co-supervisor(s) (Name, Email, Phone)		
Monash Head of Dept/Centre (Name,Email)	Mark M. Banaszak Holl, mark.banaszakholl@monash.edu	*Full name, email*
Monash Department:	Chemical Engineering	
Monash ADGR (Name, Email)	Emanuele Viterbo, Emanuele.Viterbo@monash.edu	*Full name, email*
IITB Main Supervisor (Name, Email, Phone)	Rajarshi Chakrabarti, rajarshi@chem.iitb.ac.in,	*Full name, Email*
IITB Co-supervisor(s) (Name, Email, Phone)		*Full name, Email*
IITB Head of Dept (Name, Email, Phone)		*Full name, email*
IITB Department:	Chemistry	

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

Conformational transitions in polymer molecules are impeded by solvent molecules, and sometimes additionally by intramolecular interactions. The dissipation caused by the latter are termed as internal friction, and examples of such dissipation include the damping of protein folding, the modulation of stretching transitions in polysaccharides, and the enhancement of dissipated work in the stretch-relaxation of polymers. While the microscopic origin of internal friction is many fold, it has been broadly classified as being either of the wet or dry kind. The transition of a protein from an unfolded to its native folded state is commonly interpreted as a diffusive search process over a rugged energy landscape, and the internal friction associated with landscape roughness is typically considered to be of the wet type. A characteristic feature of wet internal friction is that it vanishes in the limit of zero solvent viscosity. On the other hand, experimental measurements of the dependence of the reconfiguration time of small proteins on solvent viscosity find a finite value in the extrapolated limit of zero solvent viscosity, indicating the presence of a solvent-viscosity-independent resistance to folding, typically denoted as dry internal friction. To date the experimental quantification of internal friction has remained challenging, while theoretical models for internal friction are in their infancy. Additionally, recent advances in modelling polymer solutions has revealed the crucial role played by fluctuating hydrodynamic interactions in determining the dynamics of polymers. Models that include both internal friction and hydrodynamic interactions are rare. Understanding the consequences of internal friction is key to understanding aspects of protein folding, the dynamics of intrinsically disordered proteins, and the transient response of polymer solutions subjected to a variety of flow fields.

References:

[1] Kailasham, R., Chakrabarti, R., & Prakash, J. R., Rheological consequences of wet and dry friction in a dumbbell model with hydrodynamic interactions and internal viscosity. J. Chem. Phys. 149(9), 094903 (2018) (available on the arXiv online repository: https://arxiv.org/abs/1805.06779)

[2] Kailasham, R., Chakrabarti, R., & Prakash, J. R. Wet and dry internal friction can be measured with the Jarzynski equality, Physical Review Research, In Press (2020) (available on the arXiv online repository: https://arxiv.org/abs/1904.07473)

Project aims

The specific objective of this project is to understand the dynamics of polymers in the dilute and semi-dilute regime, where solvent viscosity, hydrodynamic interactions and internal friction within polymers are controlling the dynamics both at equilibrium and in flow. These considerations are relevant to understanding protein dynamics in a biological cell, since proteins exist in a crowded environment in cells, and experience flow. Computer simulations of a coarse-grained polymer model will be used to carefully differentiate the influence of solvent-mediated friction on conformational dynamics, from the influence of a dissipative mechanism that is independent of solvent viscosity. The work will build on and extend recent work published by the IITB-Monash research academy student Kailasham Ramalingam [1, 2].

Expected outcomes

Specific outcomes of this project will be:

1. Enhanced understanding of “internal friction” at the intra-molecular as well as at the inter-molecular level.
2. A better understanding of polymer dynamics in the semi-dilute regime, in the presence of crowding and flow, mimicking the cell environment.
3. A computer code to describe molecular dynamics in a crowded environment.

These outcomes will result in high quality journal publications within the fields of polymer dynamics and soft matter, with exemplar outputs demonstrated in recent publications from the participating academics.

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

Describe how the project will address the goals of one or more of the 6 Themes listed above.

The dynamical behaviour of biopolymers such as proteins in a crowded environment is the key to understanding how biopolymers behave in cells. Using theory and simulation we ultimately aim at the understanding of protein dynamics in biological cells where solvent flow, crowding and internal friction are expected to play important roles. Only a combination of computer simulation and theoretical techniques can shed light on such complex dynamical process. This project will firstly enhance our ability to understand mechanisms in biological systems such as biological cells. The outcome of this project will contribute to enabling aspects of the Strategic Research Priority “Living in a changing environment” and understanding the fundamental molecular aspects of Biodiversity—all of which is essential for harnessing biomolecular processes whether in health care or biotechnology.

Capabilities and Degrees Required

List the ideal set of capabilities that a student should have for this project. Be as specific or as general as you like. These capabilities will be input into the online application form and students who opt for this project will be required to show that they can demonstrate these capabilities.

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.

N/A

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.

Computer Simulation, BioScience, Modelling and Simulation, Computational and Theoretical Chemistry