

An Indian-Australian research partnership

Project Title: **Mathematical analysis and numerical methods for multiphysics problems in diffusion and viscoelasticity**

Project Number **IMURA0963**

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Research Clusters:

Research Themes:

Highlight which of the Academy's CLUSTERS this project will address? <i>(Please nominate JUST one. For more information, see www.iitbmonash.org)</i>		Highlight which of the Academy's Theme(s) this project will address? <i>(Feel free to nominate more than one. For more information, see www.iitbmonash.org)</i>	
1	Material Science/Engineering (including Nano, Metallurgy)	1	Advanced computational engineering, simulation and manufacture
2	Energy, Green Chem, Chemistry, Catalysis, Reaction Eng	2	Infrastructure Engineering
3	Math, CFD, Modelling, Manufacturing	3	Clean Energy
4	CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control	4	Water
5	Earth Sciences and Civil Engineering (Geo, Water, Climate)	5	Nanotechnology
6	Bio, Stem Cells, Bio Chem, Pharma, Food	6	Biotechnology and Stem Cell Research
7	Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng	7	Humanities and social sciences
8	HSS, Design, Management	8	Design

The research problem

Multiphysics and multi-continuum systems are of paramount importance in many different application areas, such as medicine, engineering, or environmental sciences. Mathematical modelling and numerical simulation can certainly help to understand and predict the behaviour of the underlying systems in more detail. However, due to the inherent complexity of the coupling structures and nonlinearity of the involved equations, the mathematical analysis of the resulting models and the design of numerical methods suitable for their computational simulation, remain very far from trivial. Although many theoretical advances in understanding the mathematical properties of single-physics systems are available, their counterpart for multi-physics systems is still behind. In this project, we will be concerned with the analysis of new mathematical formulations for coupled systems, focusing the theory and the computations on the interaction problem rather than the contributing single-physics alone. Two clear goals are primary: first, we focus on the challenging aspects of solvability and regularity of the underlying continuum-based models using fixed-point theorems in non-standard functional spaces; and secondly, we address the construction and analysis of reliable and robust numerical methods whose fundamental properties (physical relevance, well-posedness, convergence, stability, accuracy, and reliability) will be rigorously established.

Studying the mathematical properties of the problems at hand will require advanced knowledge of functional analysis and operator theory, as well as some notions of nonlinear PDEs. Regarding the applicative portions of the thesis, the theoretical framework will be employed in the modelling of mechanochemical interactions based on reaction-diffusion systems, incorporating appropriate modifications so that they govern the relationship between morphogenic proteins and fibroblast concentration within deforming structures, where one can explore the stress-assisted diffusion mechanism to describe the enhanced effect of the deforming structure into the transport properties. We will advance new theoretical aspects of mixed finite element schemes, as well as other more contemporary discretisation techniques such as hybrid or virtual element methods.

Project aims

- 1) Establishing the solvability of the coupled PDE-based models. This step involves advanced theoretical techniques including fixed-point theory, saddle-point and double saddle-point abstract problems, and non-standard regularity.
- 2) Studying new physics-preserving formulations for coupled multiphysics problems. Motivating examples come essentially from two applicative problems: developmental cell biology and cardiac electromechanics, and the first goal is to select suitable models and specific setups and identify where the novelties and difficulties are.
- 3) The third step focuses on proposing novel finite element and/or virtual element schemes to solve the problems studied in points 1) and 2). We will address the rigorous analysis of important properties of the proposed methods, and then we will concentrate on both 2D and 3D descriptions and access to high performance computing resources will be needed at this step. This part of the project also deals with the incorporation of geometrical interfaces.
- 4) The last objective concerns the applicative portions of our research. It consists in employing the mathematical and numerical analysis developed in the first objectives, and address questions of more practical relevance. A close interaction with the extended collaborative network of the Monash and IITB supervisors will be fostered.

Expected outcomes

- A novel framework for the rigorous mathematical analysis of a class of coupled systems of PDEs will be provided
- New aspects of continuum models for nonlinear diffusion-elasticity problems
- Robust and efficient discretisations will be advanced and their capabilities fully tested
- Results that are validated against benchmark data
- Computational codes and theoretical preprints made publicly available in online repositories

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

Specific applications of the formalisms outlined above include growth and proliferation of embryonic cells, macroscopic interaction between cardiac muscle deformation and electrical activation, and design

and testing of smart materials. The outcomes of this project will contribute to fill the gap between advanced techniques currently employed by practitioners and the sound mathematical foundation of novel models and numerical methods. Being a highly visible subject, it is expected that the project will attract several collaborations from which the IITB-Monash Research Academy will benefit. We also foresee the possibility of building new engagements with the biomedical industrial sector. All these items have a clear relevance to the goal “Advanced computational engineering, simulation and manufacture”.

Capabilities and Degrees Required

List the ideal set of capabilities that a student should have for this project. Feel free to 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.

Degree: MSc in Mathematics

Strengths:

Functional analysis

Partial differential equations

Numerical analysis of PDEs

Positive inclination towards scientific computing

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.

Neela Nataraj, IITB Mathematics. She knows the overall topic very well and has participated already in several projects from the IITB-Monash academy.

Mark Flegg, Monash Mathematics. He is a specialist on one applicative aspect of this project.

Nikhil Medhekar, Monash Material Sciences. He is a specialist on one applicative aspect of this project.