IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

CSIRO

Project Title:	**Developing New Integrated Machine Learning and Deterministic Simulation Approaches to Computational Science**	
Project Number	IMURA0723	
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Research Clusters:

Research Themes:

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

The research problem

Define the problem

Physics based computational models offer a highly accurate means of simulating natural and industrial systems. In the case of the Discrete Element Method, particle based systems such as sands, soils and powders are modelled by considering the individual particles in the system, determining the forces at inter-particles contacts and tracking and updating the motion of each of the particles. While highly accurate, these simulations are computationally expensive and can thus be difficult to apply in circumstances where computational resources are limited or an answer from a simulation is required in a short period of time for decision making purposes. Due to the high simulation cost, therea need to optimally sample the parameter space of interest when building up a model for forecasting or decision making.

Project aims

This project will aim to create a hybrid predictive tool based on computational modelling and machine learning. Machine Learning allows a system to learn from inputted sets of data to predict outcomes and dynamically adjust when presented with new scenarios or inputs. While the training of these models can be computationally expensive and the acquisition of sufficient amounts of data at times poses a significant challenge, well trained models are generally able to execute and make predictions with high speed and low computational cost. Using an integrated approach that combines data from both experiments and physics based computational models, we will develop an automated system incorporating a machine-learning model that will via active sampling determine the best simulation data to obtain and automatically generate and analyse these new simulation cases to optimally improve predictive capability. The development of these optimal active sampling techniques and methods for incorporation of both simulated and real world data will be key focuses of the project. In this way we will efficiently develop surrogate models that can be rapidly applied to problems of interest. Specific areas of application we will consider will include virtual models of Additive Manufacturing processes (3D printing) and the assessment of new materials for use in Additive Manufacturing.

Expected outcomes

New hybrid models incorporating data from both real world experiments and simulations that are able to execute faster than pure physics based computational models and give more accurate predictions with limited real world data than machine learning approaches alone.

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

Math, CFD, Modelling, Manufacturing.
Advanced computational engineering, simulation and manufacture

This project sits at the intersection of the application of computational modelling and data science to solving real world manufacturing problems. The models we will develop will incorporate novel combinations of machine learning with particle based modelling techniques and new active sampling methodologies. This will provide new tools that are capable of greatly increasing the efficiency of computational modelling in exploring a parameter space of interest and in developing new surrogate models that can be used to give operational estimates of quantities of interest where the cost of a full particle based modelling simulation is prohibitively high.

Capabilities and Degrees Required

Undergraduate or Masters level qualification in Computer Science, Physics, Mathematics, Engineering, or a related field.

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.