IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

**Project Title:** **Novel methods for high throughput experimental design in materials optimisation**

CSIRO

**Project Number** **IMURA0206**

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| Monash Supervisor(s) | Kate Smith-Miles | *Full names and titles* |
| Monash Primary Contact: | Kate.smith-miles@sci.monash.edu.au | *Email, phone* |
| IITB Supervisor(s) | Prof.Siuli Mukhopadhyay | *Full names and titles* |
| IITB Primary Contact: | siuli@math.iitb.ac.in | *Email, phone* |
| IITB Head of Department: | Prof. Sudhir R. Ghorpade | *Name, Email,* |
| IITB Department: | srg@math.iitb.ac.in | *Full name* |

## Research Academy 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**

## The research problem

*Define the problem*

Development of a new material, product, process or technology often depends on experimental optimisation of component combinations and/or processing parameters. Current advances in high throughput experimentation methodology allow this experimentation to be increasingly thorough, expanding the domain of possible response behaviour surveyed beyond the limits of application of many classical techniques for experimental design and analysis.

The objectives of this project are therefore to:

1. Compare a number of approaches including classical DoE, various stochastic approaches (for example, evolutionary or Monte Carlo techniques) and space-filling methods, noting in particular their sensitivity to the special features characteristic of high throughput combinatorial experimentation:

- sequential batch experimentation;

- gradient techniques (where varying proportions of ingredients are mixed in a continuous, non-random manner);

- the presence of experimental error;

- objective function evaluations (primarily material property measurements) that may still be relatively expensive;

- the possibility of complex response surfaces which may not be able to be described by low order global parameterisations.

2. Develop a suitable methodology for design and analysis of modern high throughput experiments.

3. Create software implementing the new methodology.

The strategy to be followed will largely consist of computer simulation techniques (ideally a suitable physical materials development programme can be found on which to validate the methodology; this depends on funding and opportunities and is not fundamentally necessary for the scope of the PhD studies). The various methodologies can be implemented and tested on some standard simulated materials development models in the literature, expanded as necessary.

## Project aims

*Define the aims of the project*

The project aims to develop theoretical approaches to the broad problem of optimising one or more responses over a high dimensional space, subject to various types of constraints. The motivating application is optimisation of material composition and processing parameters, though the same problem is encountered also in other fields. Features common to many fields include experimental error, expensive objective function evaluations, evaluated via sequential batch processing, with complicated response surfaces. Broadening optimisation techniques to handle these features would thus be useful in a range of applications.

## Expected outcomes

*Highlight the expected outcomes of the project*

1. Development of methodology appropriate to high throughput experimental materials development.
2. Insight into optimisation and search methods and development of adaptations that improve their application to problems of this type.
3. Creation of software using new methodology to generate experimental designs (and perform analysis of results where this is non-standard), either as a stand-alone product or within an environment like R or Excel (which is more accessible for end users). The final form of this software will depend on the requirements of the approach chosen.

## 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 project addresses the first goal: advanced computation engineering, simulation and manufacture. Using computer simulation techniques, it explores methods of accelerating development of new materials and/or manufacturing processes. Improving efficiency in this area has benefits across many fields including process engineering and the broad gamut of materials science.

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## 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.*

The successful student will require advanced programming capabilities and an understanding of statistical modelling and statistical design of experiments. Skills or experience in optimisation techniques would also confer a distinct advantage.