

EPSRC CDT in Distributed Algorithms

PhD Project: Artificial Intelligence for Fast Discovery of Novel Materials for Healthcare

University of Liverpool

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Project Description

This project has been developed by the University of Liverpool in partnership with Unilever.

Innovation in healthcare depends critically on creating novel materials that can control and treat infection. A similar approach is required to create new hygiene products in the personal care sector. Both sectors underpin a multi-billion-pound UK economy.

There is an urgent need to accelerate the discovery of advanced materials and surfaces that can tackle emerging healthcare and personal care challenges. This project will utilise machine learning, Bayesian optimisation, AI and high-performance computing to accelerate discovery, optimisation and development of a new generation of advanced materials and products that will protect public health and ensure societal wellbeing.

The molecular world provides the armoury to combat infection and safeguard public hygiene and health. Specifically, anti-infective agents (e.g. small molecules, natural compounds, antibiotics, etc.) are incorporated within surfaces and materials to create the operational core of many advanced technologies.

This PhD will incorporate the following elements: (1) Review of existing approaches to using Gaussian Processes to solve regression problems involving descriptions of molecules as the features and existing techniques for articulating similarities between different molecules and/or sets of molecules; (2) Development of scalable Gaussian Process implementations (e.g. involving variational or distributed approaches to representing the uncertainty) and hyper-parameter estimation (e.g. using novel Sequential Monte Carlo methods) that exploit emerging many-cored compute resources to facilitate timely performance; (3) Application of these approaches in the context of Bayesian Optimisation to help answer questions pertinent to the discovery of novel materials for healthcare.

Go to the [EPSRC CDT In Distributed Algorithms](#) website.