DPhil Computational Discovery

Project Booklet 2020/21

The DPhil in Computational Discovery is a multidisciplinary programme spanning projects in Advanced Molecular Simulations, Machine Learning and Quantum Computing to develop new tools and methodologies for life sciences discovery.

This innovative course has been developed in close partnership between Oxford University and IBM Research. Each research project has been co-developed by Oxford academics working with IBM scientists. Students will have a named IBM supervisor/s and many opportunities for collaboration with IBM throughout the studentship.

The scientific focus of the programme is at the interface between Physical and Life Sciences. By bringing together advances in data and computing science with large complex sets of experimental data more realistic and predictive computational models can be developed. These new tools and methodologies for computational discovery can drive advances in our understanding of fundamental cellular biology and drug discovery. Projects will span the emerging fields of Advanced Molecular Simulations, Machine Learning and Quantum Computing addressing both fundamental questions in each of these fields as well as at their interfaces.

Students will benefit from the interdisciplinary nature of the course cohort as well as the close interactions with IBM Scientists.

Previous projects

Mapping the protein "diffusome" of bacteria by high-throughput single-molecule tracking and advanced data analysis - *Prof. Achilles Kapanides*

Combining Molecular Dynamics D with machine learning to explore cyclic peptides - *Prof Phil Biggin*

Atomistic modelling of condensed matter on a quantum computer - *Prof. Dieter Jaksch*

Revolutionising chemical synthesis with machine learning - *Prof. Fernanda Duarte*

Potential supervisors/Project area

AI/Optimization/Machine learning

Project A - Prof. Coralia Cartis - Algorithm design, analysis and implementation for linear and nonlinear optimisation, convex and nonconvex problems

Project B - Prof. Jared Tanner - Design, analysis, and application of numerical algorithms for information inspired applications in signal & image processing

Quantum Computing

Project C - Dr. Natalia Ares – using machine learning for efficient Qubit control

Project D - Dr. Neil de Beaudrap – relationship between quantum and classical computation

Life Sciences

Project E - Prof Jane Mellor - Chromatin remodelling and gene regulation in simple eukaryotes, using AI to analyse patterns of gene transcription

Project F - Prof Ilan Davis - Genetics, cell biology and biochemistry in conjunction with advanced microscopy including super-resolution and single molecule imaging as well as computational and bioinformatics methods