Course Information Sheet for entry in 2020-21
DPhil in Computational 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.

Projects accepting applications from May 2020

This course reopened in May 2020 to accept applications for entry in the 2020-21 academic year. The following projects and supervisors are available:

Project A: Algorithm design, analysis and implementation for linear and nonlinear optimisation, convex and nonconvex problems

Academic supervisor: Prof Coralia Cartis (DPhil in Mathematics); IBM co-supervisor: TBC

Project B: Design, analysis, and application of numerical algorithms for information inspired applications in signal & image processing

Academic Supervisor: Prof Jared Tanner (DPhil in Mathematics); IBM Supervisor: TBC

Project C: Using machine learning for efficient Qubit control

Academic supervisor: Dr Natalia Ares (DPhil in Materials); IBM co-supervisor: TBC

Project D: Relationship between quantum and classical computation

Academic supervisor: Niel de Beaudrap (DPhil in Computer Science); IBM co-supervisor: TBC

Project E: Chromatin remodelling and gene regulation in simple eukaryotes, using AI to analyse patterns of gene transcription

Academic supervisor: Prof Jane Mellor (DPhil in Biochemistry); IBM Supervisor: TBC

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

Academic supervisor: Prof Ilan Davis (DPhil in Biochemistry); IBM co-supervisor: TBC

Projects accepting applications until Friday 24 January 2020

The following projects and supervisors accepted applications until 12:00 midday (UK time) on Friday 24 January 2020:

Project 1: Mapping the protein "diffusome" of bacteria by high-throughput single-molecule tracking and advanced data analysis

Academic supervisor: Prof Achillefs Kapanidis (DPhil in Condensed Matter Physics); IBM co-supervisor: Dr Simon Colgate

Protein mobility and spatial distribution inside single living bacteria can be explored by single-molecule tracking, uncovering novel information about modes of interactions of proteins in the crowded bacterial cytoplasm. We propose to massively expand our analysis to >1000 bacterial proteins with diverse functions. IBM will support the project via their know-how in algorithms, data analytics, and machine learning.

Project 2: New paradigms for AI-based multidimensional biomedical big-data exploration

Academic supervisor: Prof Ilan Davis (DPhil in Biochemistry); IBM co-supervisor: Dr Flaviu Cipcigan

This project aims to build a new standard for holding multi-dimensional and multimodality informatics and bio-imaging data on GPUs, as a model for clinical genetic and diagnostic data for near instant access and exploration. We aim to develop new paradigms for user interface and conduct exploration of these integrated data sets using the latest cloud computing, gaming technologies and machine learning methods.

Project 3: Combining MD with machine learning to explore cyclic peptides

Academic supervisor: Prof Philip Biggin (DPhil in Biochemistry); IBM co-supervisor: Dr Flaviu Cipcigan

Many diseases cannot be drugged using current small molecule therapeutics and therefore new approaches are urgently needed. One such approach that shows promise is to use cyclic peptides. The aim of this project is to understand the conformational landscape of short cyclic peptides and devise design principles using machine learning for improving pharmacokinetic properties.

Project 4: Development of training algorithms for predicting gene expression outcomes from the distribution of RNA polymerase on genes

Academic supervisor: Prof Jane Mellor (DPhil in Biochemistry); IBM Supervisor: Prof Lior Horesh

The processing, nuclear export and stability of the RNA molecules are pre-determined before transcription. We will use simulated profiles for nascent transcription over human genes to train an algorithm to predict mechanisms and parameters of transcription and gene expression, allowing all the downstream processes to be predicted without experimental determination of each stage.

Project 5: Atomistic modelling of condensed matter on a quantum compute

Academic supervisor: Prof Dieter Jaksch (DPhil in Condensed Matter Physics) and Prof Charlotte Deane (DPhil in Statistics); IBM co-supervisor: Prof Jason Crain and Dr Vadim Elisseev

The description of multipolar quantum fluctuation is a high-dimensional intrinsically complex many-body problem. In this project, we will develop quantum computing algorithms to start tackling such problems and implement them on the current generation of IBM quantum computers. Hardware specific solutions that utilise the available hardware architectures optimally will be developed.

Project 6: Revolutionising chemical synthesis with machine learning

Academic supervisor: Prof Fernanda Duarte (DPhil in Organic Chemistry); IBM co-supervisor: TBC

This project aims to accelerate the discovery of complex drugs and materials by combining organic chemistry principles, quantum chemistry, and machine learning. It will focus on the development of interpretable models that can not only lead to the discovery of new drugs but also provide an understanding of challenging processes leading to their formation and mode of action.

Project 7: Optimisation methods for machine learning

Academic supervisor: Prof Coralia Cartis (DPhil in Mathematics); IBM co-supervisor: Prof Lior Horesh, Dr Soumyadip Ghosh, Dr Songtao Lu

Optimisation problems, of huge scale, form the modelling and numerical core of machine learning and statistical methodologies. A grand challenge in this area is the need to augment stochastic gradient optimisation methods with inexact second-order derivative information, so as to obtain more efficient methods especially in the nonconvex case of deep learning. In this project, we will investigate ways to approximate second-order information in the finite-sum structure of ML optimisation problems.

Project 8: Compiling chemistry / optimisation problems to higher-level anharmonic oscillators

Academic supervisor: Niel de Beaudrap (DPhil in Computer Science); IBM co-supervisor: TBC

This project aims to develop techniques to break down optimisation problems and other problems, using building-blocks consisting of higher-level interactions in superconducting quantum systems.

Project 9: Optimising qubit control with machine learning

Academic supervisor: Dr Natalia Ares (DPhil in Materials); IBM co-supervisor: Dr Ali Javadi-Abhari

This projects aims to achieve automated tuning of semiconductor qubits encoded in gate-defined quantum dots and to use a machine learning approach to enable the tuning of large quantum circuits.

Project 10: New paradigms for dissecting those “black-box” AI models

Academic Supervisor: Prof Jared Tanner (DPhil in Mathematics); IBM Supervisor: Dr. Payel Das and Dr. Pin-Yu Chen

Understanding deep learning (DL) models is of critical importance, as a framework to explain black-box models will chart a path to trustworthy AI. Neural network training relies on the ability to find “good” minimisers of highly non-convex loss functions. There is an urgent need to develop new theoretically grounded framework that can automatically and efficiently decipher the structure-performance (both in terms of generalisation and robustness) of NN models. A similar framework is also needed to understand the impact of hyperparameter settings on model performance, as it is known that well- chosen training parameters (batch size, learning rate, optimiser) produce minimisers that generalise better. Finally, the framework will allow developing models capable of multi-task and multi-environment learning.

Project 11: New paradigms for combining AI and Molecular Simulations for Accelerated Discovery

Academic Supervisor: Prof Philip Biggin (DPhil in Biochemistry); IBM Supervisor: Dr. Payel Das

Data-driven approaches including Machine learning (ML) and deep learning (DL) have shown incredible promises for accelerating scientific discovery in domains such as biology, chemistry, and material science. On the other hand, molecular simulations have come up a long way and being routinely used as a complement or supplement to experiments for validating predictions and providing mechanistic insights to complex processes. There is an urgent need to develop new technology paradigms for automatically and efficiently:

1. including the feedback from simulations in order to improve the ML model;
2. optimising the need for additional expensive simulations; and
3. identifying hidden features from the cheaper simulations that can be a good proxy to learning from expensive simulations.

After a very short induction period of one or two weeks, during which some basic training is provided, you will start a research project in your academic supervisor's laboratory.
Your supervisor may appoint a senior member of the laboratory as your day-to-day supervisor. Most laboratories have weekly meetings where members present and discuss their research results with other members of the laboratory. You will also regularly present your work in progress seminars, which are attended by other research groups working in related areas. Further support is available from your college advisor.

There are a number of key stages in the research programme:

1. Within a month of starting, you will meet with your academic and IBM supervisors to finalise your project and agree on an initial programme of research.
2. Within the first three months, you will complete an analysis of your training needs with your academic supervisor.
3. After just under one year you will apply to transfer to DPhil status. To do this you write a report describing your research to date and plans for the future. This will be assessed by two independent experts, who interview you as part of the process.
4. You will apply to confirm your DPhil status by the end of your third year. This involves writing a short progress report and thesis outline and giving a presentation. The application is assessed by two experts.
5. The final stage is submission of your DPhil thesis, which needs to be done within four years.

Whilst working on your research project you will participate in a comprehensive, flexible skills training programme which includes a range of workshops and seminars in transferable skills, generic research skills and specific research techniques. There are also numerous seminars and lectures by local and visiting scientists and you are provided with many opportunities to meet leading scientists.

Supervision

The allocation of graduate supervision is the responsibility of the Medical Sciences Graduate School and it is not always possible to accommodate the preferences of incoming graduate students to work with a particular member of staff. Under exceptional circumstances a supervisor may be found outside the department leading the course.

Changes to courses

The University will seek to deliver this course in accordance with the description set out above. However, there may be situations in which it is desirable or necessary for the University to make changes in course provision, either before or after registration. For further information, please see the University's Terms and Conditions.

Expected length of course

Mode of study	Full Time Only
Expected length	3 to 4 years

Costs

Annual fees for entry in 2020-21

Fee status	Annual Course fees
Home/EU (including Islands)	£7,970
Overseas	£26,405

Course fees are payable each year, for the duration of your fee liability (your fee liability is the length of time for which you are required to pay course fees). For courses lasting longer than one year, please be aware that fees will usually increase annually. Information about how much fees and other costs may increase is set out in the University's Terms and Conditions.

Course fees cover your teaching as well as other academic services and facilities provided to support your studies. Unless specified in the additional cost information (below), course fees do not cover your accommodation, residential costs or other living costs. They also don't cover any additional costs and charges that are outlined in the additional cost information.

Graduate students who have reached the end of their standard period of fee liability may be required to pay a termly University and/or a college continuation charge.

The University continuation charge, per term for entry in 2020-21 is £508, please be aware that this will increase annually. For part-time students, the termly charge will be half of the termly rate payable by full-time students.

If a college continuation charge applies (not applicable for non-matriculated courses) it is likely to be in the region of £100 to £400 per term. Please contact your college for more details.

Additional cost information

There are no compulsory elements of this course that entail additional costs beyond fees (or, after fee liability ends, continuation charges) and living costs. However, please note that, depending on your choice of research topic and the research required to complete it, you may incur additional expenses, such as travel expenses, research expenses, and field trips. You will need to meet these additional costs, although you may be able to apply for small grants from your department and/or college to help you cover some of these expenses.

Living costs

In addition to your course fees, you will need to ensure that you have adequate funds to support your living costs for the duration of your course.

The likely living costs for 2020-21 are published below. These costs are based on a single, full-time graduate student, with no dependants, living in Oxford. We provide the cost per month so you can multiply up by the number of months you expect to live in Oxford.

	Likely living costs for 1 month		Likely living costs for 9 months		Likely living costs for 12 months	
	Lower range	Upper range	Lower range	Upper range	Lower range	Upper range
Food	£270	£385	£2,430	£3,465	£3,240	£4,620
Accommodation	£630	£760	£5,670	£6,840	£7,560	£9,120
Personal items	£130	£245	£1,170	£2,205	£1,560	£2,940
Social activities	£45	£110	£405	£990	£540	£1,320
Study costs	£40	£95	£360	£855	£480	£1,140
Other	£20	£55	£180	£495	£240	£660
Total	£1,135	£1,650	£10,215	£14,850	£13,620	£19,800

When planning your finances for any future years of study at Oxford beyond 2020-21, you should allow for an estimated increase in living expenses of 3% each year.

More information about how these figures have been calculated is available at www.graduate.ox.ac.uk/livingcosts.