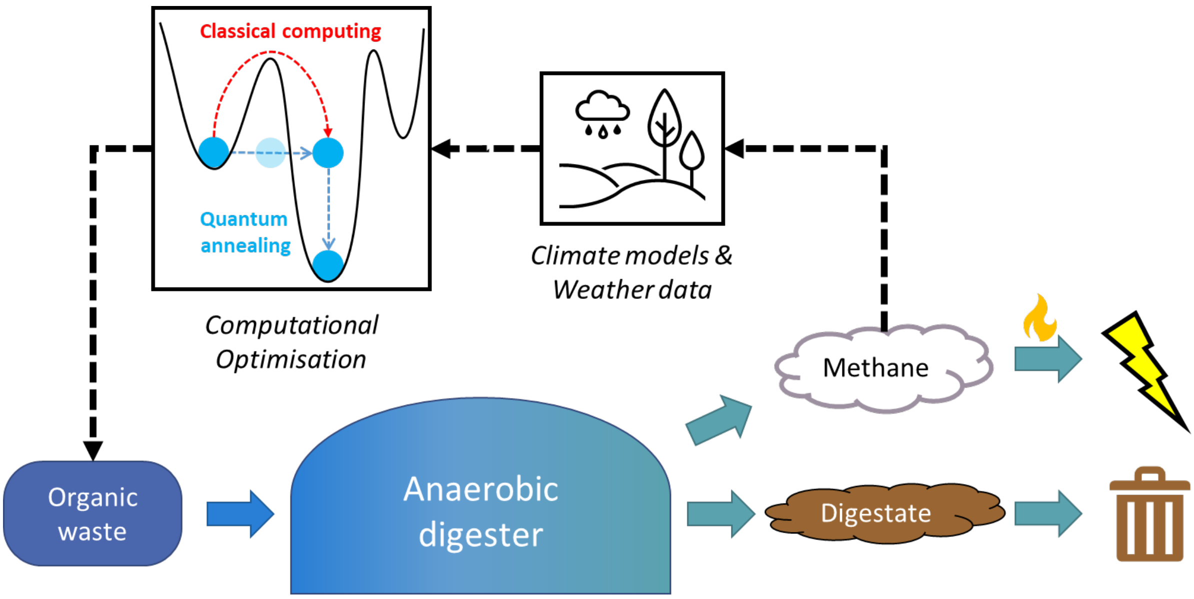
Title

Quantum Annealing for Simulation Optimisation with Applications in Climate Systems and Wastewater-driven Energy Facilities



Challenge

Many real-world systems - including climate systems and wastewater-to-energy production using anaerobic digesters in wastewater treatment (WWT) - are far too complex for closed-form mathematical expressions to adequately describe, necessitating time-consuming, computer simulations to analyse and predict their behaviour. Rather than limited - and incomplete - scenario analysis of classical simulated systems, we propose to take an optimisation approach (even if optimisation is not the primary objective), to identify the set of initial conditions and/or model parameter values that predict extreme outcomes (positive or negative) accurately. In this regard, we seek to apply quantum annealing algorithms for speeding up such computational-demanding tasks.

In previous research, we introduced QuAnCO (Quantum Annealing Continuous Optimisation), an adaptation of Trust Region Newton (TRN) which enables the use of Ising solvers such as D-Wave's quantum annealers for solving the Trust Region (TR) subproblem. However, the original QuAnCO algorithm is limited to unconstrained, continuous optimisation of smooth - i.e., twice differentiable - objective functions. Our goal is to extend QuAnCO to solve optimisation problems with 1) equality and inequality constraints, 2) a mix of continuous and discrete parameters, and/or 3) objective functions which lack the second (or even the first) derivative(s). Such extensions would allow us to solve a wider range of optimisation problems, such as simulating the climate and WWT systems we proposed. This project could surpass the classical quality of sensitivity analyses and ultimately lead to more effective quantum solutions for renewable energy and environmental sustainability.

Project

To recap the previous section, in this project, we pursue two overarching objectives:

1. Expanding the applications and impact of quantum computing (specifically, quantum annealing) in solving optimisation problems, and
2. Improving the quality of sensitivity analyses done for simulated systems, including climate models and wastewater treatment reactors (which use anaerobic digestion for generating biomethane from wastewater).

Our efforts will be focused on 1) expanding QuAnCO, 2) adapting climate models for optimisation, and 3) investigating the impact of weather on Wastewater-to-energy operations. In each area, we will perform exploratory / proof-of-concept work, within the time constraints of the seed grant, to validate/refute the key assumptions in our framework and shape future research directions.

Expanding QuAnCO

QuAnCO will be extended to handle 1) linear/nonlinear equality/inequality constraints, 2) objective functions without the Hessian or gradient, and 3) parameter spaces that are a mix of continuous and discrete parameters. The initial focus will be on literature review, validating the initial strategies for each case, implementing basic versions of the algorithms, and limited testing of the algorithms.

Adapting Climate Models for Optimisation

We will identify the state space of major climate models, and explore how sensitivity analysis of these climate models can be translated into optimisation problems. We will also explore various options (including the computational infrastructure and software wrappers needed, as well as expected runtimes) for running these models as part of a larger optimisation process.

Impact of Weather on Wastewater-to-energy Operations

We will explore the available data for WWT facilities in the UK to identify modelling possibilities and limitations as well as operational challenges that could be translated into optimisation formulations. We will perform exploratory analysis of available weather, in conjunction with wastewater operational data, to identify potential correlations between climate trends and operational metrics of these facilities. Combining models that predict WWT operations from climate data with climate models that predict the range of possible climate outcomes in the future would allow us to perform sensitivity and optimisation analysis on a combined model that reflects the range of possible outcomes in WWT operations as a function of climate change.

Researchers Involved

Mansour T.A. Sharabiani

Mansour has conducted research on applying quantum computing to renewable-energy problems, specifically anaerobic digestion in biogas reactors. Focusing on a high-dimensional, biomass-selection optimisation problem from Nature Energy - the largest biogas producer in Europe, recently acquired by Shell for two billion dollars - he invented a new framework, QuAnCO, enabling continuous optimisation problems to be solved by quantum annealing. He presented his work as an invited speaker at D-Wave Qubit 2021 Conference. Mansour was a roundtable panellist for the IEEE Quantum Computing Climate Change Summit. Mansour has been actively engaged in solving real-world problems in areas such as deep learning solutions for the analysis of Synthetic Aperture Radar (SAR) imagery. One of Mansour's areas of focus in scientific computing research has led to the development of a high-performance, parallelisation framework - along with implementation in C - for estimation of Bayesian models that offers a 5-fold speedup over the multithreaded Intel MKL library (see paper). He has developed a number of statistical software packages including, but not limited to, R packages for ensemble machine learning (EnsembleBase, EnsembleCV, EnsemblePCReg, EnsemblePenReg), Bayesian mixture survival modelling (BayesMixSurv, BSGW), competing risk analysis (CFC), Markov Chain Monte Carlo sampling techniques (sns, MfUSampler), and an optimised C++ class for Single-Instruction, Multiple-Data (SIMD) random number generation (arxiv paper). Mansour leads the Machine Learning specialisation for the GMPH programme; he also co-leads the Advanced Statistics & Data Science specialisation for the MPH programme.

Po-Heng (Henry) Lee

Henry has deep expertise in engineered waste-to-energy anaerobic digestion optimisation. His research leverages microbial anaerobic digestion structure metabolism and its full-scale facilities for procrastinating and optimisation. His state-of-art research techniques developed include quantum computing using IBM Qiskit (e.g., Quantum Information Theory, Variational Quantum Eigensolver), and hybrid meta-omics techniques. This new method enables the identification of new operating parameters in engineered anaerobic digesters, enabling a healthy environment. He will provide an 8-year full-scale AD dataset, including operation and microbial genomic information for this project. PL has held over £1.5M funding as PI from prestigious awarding bodies including UK EPSRC, UK UKRI, and HK University Grants Committee, as well as consulting projects for UK Jacobs, SUEZ Environment, HK Drainage Services Department, and CLP Power HK Limited. He is a member of the Wastewater and Biosolids Management panel of the UK Chartered Institution of Water and Environmental Management (CIWEM).