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Project 1: Quantum control engineering with trapped ytterbium ions

Keywords: Quantum computation, Quantum Simulation, Quantum Control

The development of well-controlled quantum systems for computational purposes is one of the most promising avenues to unlock solutions to hard and often intractable problems in areas ranging from chemistry and materials science to physics.

While much progress has been made over the last decades, further improvements to the performance of quantum operations are required to turn small proof-of-principle demonstrators into reliable quantum computers and simulators that produce results even in the presence of unavoidable noise perturbing the quantum system.

In this project, we use the most advanced trapped-ion quantum computing platform in Australia to experimentally realize novel quantum control schemes that are specifically tailored to suppress noise in quantum operations, aiming to bridge the gap to near-term usefulness by combining quantum physics with control engineering approaches.

Classical electrical engineering uses a variety of techniques to characterize the time-domain evolution of control pulses and their corresponding representation in frequency space. This approach, known as the filter-function formalism, allows one to predict the performance and noise-susceptibility of control processes. In the quantum domain, a similar framework can be established and has been underpinning the research at the Quantum Control Laboratory for several years, yielding many contributions in both theory and experiment.

Our experimental work is carried out using trapped ytterbium ions that encode quantum information in their internal hyperfine energy levels, which we manipulate using microwave and laser radiation. With phase coherence times beyond one second, ytterbium ions are among the best performing quantum bits available, offering a chance to work at the cutting-edge of what is technologically possible.

This project will develop and use techniques to characterize both environmental noise and disturbances that are intrinsic to our control pulses. You will then craft special modulation sequences that change their frequency, amplitude and phase to suppress the detrimental effects of the noise and allow for an improved performance of the desired operation.

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Expected outcomes are both a full characterization of the error robustness of the augmented quantum operations as well as their use in a demonstration of superior performance in an application targeting a specific problem of interest, e.g. the experimental quantum simulation of chemical reaction.

Supervisor: Dr Cornelius Hempel

School of Physics

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Additional Supervisor: Professor Michael Biercuk

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Project 2: Conserved Regulatory Genes in Neurodevelopment

Keywords: Stem cells, Organoids, brain development, human

The present project aims to utilize the promising combination of 3D organoid technology and CRISPR genome editing, which will allow us to examine the roles of several conserved genes involved in neurodevelopmental regulation, in order to better understand human neuronal development at the molecular level. Investigating these mechanisms can not only shed light on human brain development, but also lead to new treatments for neurological diseases.

Insight into the roles of conserved regulatory genes will provide a strong frame work for the understanding of developmental and morphogenic characteristics related to neurodevelopmental disorders. To examine the role of our candidate genes in neurodevelopment, we intend to utilize CRISPR genome-editing to knockout conserved neuronal regulator genes in human-derived 3D brain organoids. This will enable us to assay the functional roles of the respective genes during neurodevelopment by examining cell morphology and phenotype, neuronal firing activity and synaptic connectivity of an intact tissue. The proposed research aspires to understand paramount mechanisms in human neurodevelopment as well as in neurodegeneration.

Supervisor: Associate Professor Greg Neely

School of Life and Environmental Sciences

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Additional Supervisor: Associate Professor Greg Sutherland

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Project 3: Controls on the Holocene evolution of the Great Barrier Reef: linking 4D numerical modeling and observational data

Keywords: Great Barrier Reef, reef geology, numerical modeling, sea level and climate change

This project will investigate the biological and geological processes that control the evolution of coral reef systems (e.g. reef communities, stratigraphic ages and growth rates, reef geometries ('architecture'). We will construct new 4D numerical models using state of the art software (e.g., pyReef, pyBadlands) and compare them against rich observational reef data sets from the Great Barrier Reef (GBR) that grew during the Holocene (10,000 years to now). We aim to assess the sensitivity of coral reef systems to various environmental stresses (e.g. sea-level rise, hydrodynamic energy, sediment flux) acting on different timescales, magnitudes and rates. The project may also involve field work to One Tree Reef/Heron in the southern GBR to calibrate model parameters and processes against real world sedimentary and biological examples.

Predicting how the GBR will respond in the face of future global climate changes is both poorly constrained and controversial. This relates to our incomplete understanding of how reef systems respond to environmental changes but also the lack of baseline data — particularly on centennial to millennial time scales. In this project, you will integrate existing sedimentologic, biologic, geochemical, and chronological data sets from a unique suite of fossil reef cores recently collected from the southern GBR. Then you will use sophisticated modelling software (pyReef-Core, pyBadlands) that predicts reef core stratigraphy, facies, communities and geometries, and in combination with innovative data sciences tools (Bayes Reef - Bayesian inference computational algorithm) to optimize model inputs/parameters, to explore the past evolution of the GBR in response to major global climate and environmental changes. This will improve our understanding of the sensitivity of the GBR to multiple environmental stresses and help improve predictions about the future fate of the reef. This project is part of a new $4 million ARC Industrial Transformation Training Centre grant called DARE (Data Analytics for Resources and Environments Centre) and will enable researchers and PhD students to apply their data science models against real world challenges, such as water storage, biodiversity loss and the extraction of mineral resources.

https://sydney.edu.au/news-opinion/news/2019/08/27/4-million-for-data-science-research.html

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The PhD candidate will work closely with other DARE project members, as well as the extensive network of national and international collaborators of the Geocoastal Research Group (GRG) - https://grgusyd.org/.

Supervisor: Associate Professor Jody Webster

School of Geosciences

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Additional Supervisor: Dr Tristan Salles and Dr. Rohitash Chandra

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Project 4: Reconstruct trans-regulatory networks using multi-omics profiling and data integration

Keywords: cell regulatory networks, computational models, omics data

A major initiative in our group is to integrate trans-omics datasets generated by a state-of-the-art mass spectrometer (MS) and next-generation sequencer (NGS) from various cell systems. We have now profiled various stem/progenitor cell differentiation processes using a combination of MS and NGS and have generated large-scale trans-omics datasets in these cell systems (see https://doi.org/10.1016/j.cels.2019.03.012. These data provide exciting research directions where we hypothesize that data integration across multiple omics layers is the key to a comprehensive understanding of the underlying biological systems.

The aim of this PhD project is to develop computational methods for integrating and making sense of multi-layered omics datasets. Specifically, you will be developing and applying unsupervised, semi-supervised and supervised machine learning techniques and general data analytics for integrating and making sense trans-omics data that capturing the dynamics of stem and progenitor cell differentiation. Programming skill is essential for this project. Knowledge discovered from this project will translate into exciting biological findings and shed light on development, regeneration, and treatment for complex diseases and aging.

Supervisor: Dr Pengyi Yang

School of Mathematics and Statistics

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Project 5: LSTM-GANs: Generation and Missing Value Imputation for Time Series Multi-Omics Data

Keywords: Deep learning, computational models, multi-omics, imputation, time series

Biological processes are often dynamic, and thus researchers often monitor their activity at multiple time points. The most abundant source of information regarding such dynamic activity is time-series gene expression and proteomics data. These data are used to identify the temporal patterns of activated genes in a biological process, to infer their rates of change, their order and their causal effects and to model dynamic systems in a cell. However, the analysis of time-series omics data could be complicated by various challenges such as missing values. Developing effective computational methods to overcome the difficulties associated with time-series data analysis is critical.

This project aims to develop and utilise a novel deep leaning method which can generate and impute missing values for time series omics data. Temporal omics data, such as RNA-seq, proteomics, phosphoproteomics and epigenomics are essential to discover complex biological interactions and clinical mechanism. While they are useful for analysing temporal dynamics of biological systems, they often suffer from missing-value problem due to a variety of biological and experimental reasons. To overcome this problem, we will investigate the utility of an unsupervised method based on Generative Adversarial Networks (GANs) for time-series data imputation. By using Long-Short-Term-Memory Recurrent Neural Network (LSTM-RNN) as the generator and discriminator in the GAN framework to capture the temporal correlation of time series omics data distributions, we aim to estimate missing entries for high dimensional time series omics data and to generate synthetic datasets. Time series single-cell RNA-sequencing (scRNA-seq) will be our entry point for the algorithm and the model will be extended for other time series omics data generation/missing value imputation.

Supervisor: Dr Pengyi Yang

School of Mathematics and Statistics

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Project 6: Automated Chemical Synthesis of Proteins in Flow

Keywords: solid-phase peptide synthesis, peptide ligation, flow chemistry, peptide, protein

Peptides and proteins underpin most biological processes in nature. Understanding these biological processes requires an understanding of peptides and proteins, and by extension their precise structure and function. The ubiquity of proteins in biological processes, as well as their exquisite target selectivity, makes them excellent therapeutic candidates as highlighted by the fact that they have double the success rate for FDA approval when compared to small molecules. However, the current study of peptides and proteins, especially those bearing post-translational modifications, has been hampered by a lack of methods that can reliably access them in pure form.

Many peptides and proteins can be accessed through recombinant techniques, whereby the cellular machinery of natural systems used to produce polypeptides. While this is an incredibly powerful technique that can access large quantities of proteins, the ability to include non-proteinogenic amino acids or modifications is limited. The underpinning chemical method to access peptides is solid-phase peptide synthesis (SPPS) and led to the award of the 1984 Nobel Prize to Merrifield.9 However, peptides greater than 40 amino acids in length cannot be generated via this method. A key strategy to overcome the size limitation of SPPS is the convergent fusion of peptide fragments by native chemical ligation (NCL, Dawson et al. Science 1994). NCL is a reaction which occurs chemo selectively between two fully unprotected peptide fragments, one bearing an N-terminal cysteine residue and the other a C-terminal α-thioester moiety. Despite the utility of NCL in protein synthesis, the need for an N-terminal Cys residue at the ligation site limits the possible retrosynthetic disconnections which can be considered, especially given the rarity of cysteine in proteins (1.8% abundance). Given that some proteins either do not contain cysteine or do not possess this residue at synthetically useful junctions, this renders some polypeptides inaccessible by NCL. To overcome this limitation the Payne and co-workers have developed ligation-desulfurization chemistry at 10 different proteinogenic amino acids that has expanded the scope of ligation chemistry and the number of targets that can be accessed through chemical synthesis (see Payne et al. Nature Rev. Chem. 2018).

The Payne lab has recently described the first flow-based manifold for performing rapid and efficient one-pot ligation-photo desulfurization chemistry (Chisholm et al. JACS, 2018). The aim of this project will be to capitalize on this initial discovery for the development of new technologies that enable the rapid,

automated and efficient synthesis of a large range of important peptide and proteins, including therapeutics. The following two areas of investigation will serve as the initial focus:

Diselenide-selenoester ligation (DSL), a novel ligation strategy developed in the Payne group will be coupled to a novel photo-desalinization methodology for the first time in flow. This will then be used in concert with NCL to enable one-pot tandem NCL-DSL reactions which will enable access to larger proteins. NCL and DSL methodologies will be investigated at high dilution in flow. The enhanced mixing in flow may lead to accelerated rates of ligation relative to hydrolysis, allowing for a broader range of targets to be accessed. Targets containing highly hydrophobic regions, including integral membrane proteins may be synthesised that would be otherwise inaccessible by batch methods due to limited solubility.

A key methodology for this project will be the use of SPPS to synthesise peptide fragments for developing peptide reaction methodology in flow. This synthetic methodology is by far the most effective in synthesising peptide fragments. Flow apparatus (available in the Payne lab) will be used to perform reactions in flow under a range of conditions, including UV and visible-light irradiation. Flow chemistry can provide a range of benefits over traditional batch chemistry, and photoirradiation has previously been demonstrated to be useful in accelerating peptide reaction processes. Peptide targets will be purified by RP-HPLC and analysed by UPLC, LC-MS, and MALDI-TOF, all standards in the field. These analytical techniques can be used to monitor reaction rates and accurately characterise target proteins. The use of UPLC to monitor reaction rates is particularly useful due to the excellent separation and accurate absorbance measurements provided. Characterisation of the synthetic proteins will involve a suite of spectroscopic and biophysical techniques, including NMR, CD, ITC and SPR. The project will also involve the development of in vitro assays to assess biological activity. All in vivo assays will be performed in collaboration with Novo Nordisk (Copenhagen).

Supervisor: Professor Richard Payne

School of Chemistry

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Project 7: Exploring the Sulfoproteome using Synthetic Sulfoproteins

Keywords: solid-phase peptide synthesis, peptide ligation, peptide, protein, sulfation

More than 70% of all mammalian proteins are predicted to be functionalised with posttranslational modifications (PTMs). These modifications serve to expand the functional repertoire of proteomes by altering structure, activity and stability; yet, surprisingly, the identities and precise roles of PTMs are unknown for most proteins. Tyrosine (Tyr) sulfation is a PTM of secreted and transmembrane proteins that plays a pivotal role in physiological processes by modulating protein-protein interactions, e.g. in blood coagulation, inflammatory and immune responses orchestrated by chemokine signaling and viral entry. Several sulfopeptides from invertebrate sources have also gained prominence as therapeutic leads, e.g. anticoagulant proteins from medicinal leeches. Despite the undeniable importance of Tyr sulfation in these examples, both the presence of the modification and its functional consequences remain poorly characterised compared to other PTMs (e.g. glycosylation and phosphorylation). In order to better understand Tyr sulfation we desperately need new tools to rapidly and efficiently produce homogeneously sulfated proteins (sulfoproteins).

The Payne lab has recently developed new peptide ligation methods that provide a viable route to small sulfated proteins (80-90 residues). The challenge now is how to construct larger sulfoprotein targets (>90 residues). In this PhD project you will use cutting-edge ligation technologies and photochemical transformations for the rapid and efficient synthesis of homogeneous sulfoprotein libraries, not accessible by any other means. These methodologies will be used to synthesise two different classes of proteins. Specifically, the aim will be to:

- (A) Develop a novel strategy to synthesise a library of homogeneously sulfated single chain antibodies (nanobodies) and evaluate the effect of sulfation on the affinity and selectivity of their chemokine binding.
- (B) Uncover the role of Tyr sulfation on the activity, selectivity and stability of anticoagulants from tick saliva via the assembly of a panel of differentially sulfated peptides and proteins.

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The PhD project is interdisciplinary in nature and will require a combination of synthetic organic chemistry, solid-phase peptide synthesis, peptide ligation chemistry, biochemistry and chemical biology. There are two classes of sulfated protein target that will be generated by chemical synthesis in the project which are summarized below:

1. Chemokine-targeting nanobodies contain Tyr sulfation motifs:
   Recently, several chemokine-binding nanobodies (Nbs) were discovered through immunisation of llamas with specific human chemokines followed by selection of functional Nbs through phage display. Nbs are small (12-15 kDa) VHH single chain antibodies that possess one or two disulfide bonds, and three variable complementarity-determining regions (CDR1, CDR2 and CDR3) that facilitate antigen binding (Fig. 2). Candidate Nbs that bound to a range of inflammatory chemokines, including CCL5, CCL3, CCL2, CXCL12 and CXCL11, were elucidated with affinities in the high pM to low nM range. However, the presence of PTMs within the CDRs has not been investigated.
   Like natural virus and tick chemokine binding proteins, the key CDRs possess a number of Tyr residues that would be sulfated in vivo and would likely affect both affinity and selectivity. In this project you will use cutting-edge synthetic technologies to prepare homogeneously sulfated variants of five Nbs to assess the effect of the PTM on the affinity and selectivity for a variety of chemokines as well as signaling and chemotaxis.

2. Blood Feeding Organisms Produce Sulfated Anticoagulants:
   Tyr sulfation drastically enhances the activity and stability of anticoagulant proteins from blood feeders: Hematophagous organisms, such as leeches and ticks, have evolved highly effective mechanisms to facilitate the acquisition of a blood meal via the production of exquisitely potent and selective inhibitors of host coagulation factors, the enzyme thrombin. One feature of these molecules that is almost always overlooked is the presence of PTMs and the effect they may have on activity and/or stability. Indeed, even though the clinically approved recombinant anticoagulant hirudin is unmodified, the family of native leech proteins is sulfated, and the modification has been shown to impart a 10-fold improvement in thrombin inhibitory activity.

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My group has recently revealed an important role of Tyr sulfation for the thrombin inhibitory activity of two saliva derived thrombin inhibitors - madanin-1 and chimadanin - from the bush tick Haemaphysalis longicornis (Nature Chemistry, 2017). Both proteins were predicted to be sulfated based on the presence of two conserved Tyr residues within an acidic stretch of amino acids. To test this prediction the proteins were expressed in insect cells (baculovirus) which showed heterogeneous sulfation at the predicted sites. Synthetic homogeneously sulfated variants of the two proteins were then generated through cutting-edge ligation methods and demonstrated that sulfation enhances thrombin inhibitory activity (Ki = 0.41 nM for doubly sulfated vs 210 nM for unsulfated chimadanin). This improved potency resulted from electrostatic interactions between the sTyr residues and conserved Lys residues on exosite II of thrombin which was confirmed by X-ray crystallography. Based on these findings we now hypothesise that Tyr sulfation is a widespread modification of salivary proteins from other ticks that could serve as a general mechanism for modulating anticoagulant activity during feeding and/or improving stability. You will test this hypothesis in this project by investigating a new class of thrombin-inhibiting tick sulfopeptides and sulfoproteins using a combination of chemical protein synthesis and rapid anticoagulant screening methods.

Supervisor: Professor Richard Payne

School of Chemistry

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Project 8: Ground-state cooling and high-fidelity detection of large ion crystals in a Penning trap for quantum simulations

Keywords: Quantum simulation, ion trapping, atomic physics, laser systems

The understanding of the dynamics of many-body quantum systems is one of the most challenging problems in physics today. Advancing our knowledge of these systems can lead to significant benefits in the understanding of condensed matter phenomena such as high-temperature superconductivity and spin liquids but also enable insights into dense astrophysical matter as found e.g. in neutron stars. |To gain controlled access to these systems and engineer their interaction, we are using some of the most precise tools in atomic physics, the Penning ion trap and laser systems, to build and investigate multi-particle systems ion by ion.

The controlled simulation of dynamics in quantum-many body systems is of central interest in the pursuit to further our understanding of condensed matter phenomena. Specially designed Penning ion traps enable experimental investigations into these topics using hundreds of ions trapped simultaneously. We have recently brought online the first and only such system in Australia at the Sydney Nanoscience Hub and now routinely trap large crystals of beryllium ions. The focus of the work is on finalizing the setup of the laser-based beryllium qubit manipulation and implementing software-based state analysis. Lasers near 313nm are used to address electric dipole transitions in beryllium ions. These transitions can be used to effectively Doppler laser cool an ensemble of ions to ~1mK temperature, such that it forms an ion crystal - a regular and stable lattice of charged particles, formed due to the equilibrium of Coulomb repulsion and electromagnetic confinement. However, for many envisaged experiments, the residual motional temperature must be decreased even further, close to the ground state of motion.

This can be achieved by implementing so-called ground state cooling techniques using lasers with different beam geometry and characteristics. The development and setup of this system followed by the before mentioned state-of-the-art quantum simulation and metrology experiments is a possible project. To investigate correlations between individual ions, or qubits, in a quantum simulation, the spin state of the ion must be read out. This is accomplished by detecting the ion's fluorescence photons. Ion crystals in a Penning trap rotate in the strong external magnetic field of a superconducting magnet due the Lorentz force. Therefore, a precise correlation between photon time a position is required. The setup of

such detection systems and its integration into the existing experimental control software in combination with the development of algorithms employing machine learning is a possible project. These projects are expected to generate new knowledge in the area of quantum science and have a multitude of possible future applications in quantum technology, such as quantum scale materials, quantum sensing and quantum computation. In particular, understanding quantum magnetism is on the forefront of modern physics.

Supervisor: Dr Robert Wolf

School of Physics

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Additional Supervisor: Professor Michael Biercuk

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Project 9: The nutritional geometry of non-alcoholic fatty liver disease, cardio-metabolic health and lifespan

Keywords: nutrition, Liver, metabolism, lifespan

The global epidemic of obesity and type 2 diabetes (T2D) has been linked to increased consumption of 'western diets' containing an abundance of processed foods rich in saturated fats and 'simple carbohydrates. Furthermore, increased intake of sugars and fats promotes the development of non-alcoholic fatty liver disease (NAFLD) - the commonest form of liver disease in the Western world, affecting one in three people in the general population. Accumulation of liver fat is thought to be a principal driver of T2D, and it is usually associated with dyslipidemia, particularly increased circulating triglycerides. The fat deposition in NAFLD can be caused by an increase in endogenously synthesised fatty acids in the liver (de novo lipogenesis), by increased consumption of dietary fatty acids that are subsequently stored in the liver, or both. Using the Geometric Framework research methodology, we will investigate how different dietary nutrients affect liver biology, late-life cardiometabolic health status and longevity.

The Geometric Framework (GF) - a nutritional modelling platform - has revolutionized our capacity to interpret the complex relationship between food and phenotype. In the GF, a model of an animal's nutritional relations with its environment is constructed around an n-dimensional nutrient space (e.g. protein, carb and fat) and phenotypic parameters (e.g. fat mass) are superimposed on this space by plotting response surfaces. This allows analysis of macronutrient intake targets of animals, their feeding response to diets with different compositions, and its impact on performance characteristics. Our research using the GF has robustly shown in invertebrates and mice that diets low in protein and high in carbohydrate content generate the best metabolic health and lifespan outcomes despite increased energy intake ('protein leverage'). In this advertised project we will extend our work by investigating how the source of dietary protein (animals vs plant), fat (animal vs plant) and type of carbohydrate (simple vs complex) regulates cardiometabolic health, liver fat deposition and lifespan using the laboratory mice as a model organism. We will study how different types of carbohydrates (glucose, fructose, starch and sucrose) interact with protein and fat to drive the pathogenesis of fatty liver, obesity and insulin resistance. The study will be conducted at the Charles Perkins Centre and will include male and female mice maintained on diets with different ratios of protein, fat and carbohydrates

derived from various sources. The PhD candidate will be involved in animal husbandry, in vivo metabolic phenotyping, animal dissections and in vitro assessment of tissue health by molecular biology techniques (qPCR, ELISA, western blotting and histology).

Supervisor: Professor Stephen Simpson

School of Physics

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Additional Supervisor: Dr Jibran Wali