Trinity College School of Physics Summer Undergraduate Research Experience (SURE) 2023

PROJECT #1: Computer simulations of three-dimensional foams

Supervisor: Prof. Stefan Hutzler (https://www.tcd.ie/physics/research/groups/foams/)

Research Area:
Foams are dense packings of deformable gas bubbles, surrounded by liquid. For many purposes they serve as a model system for soft matter (such as for example emulsions or biological cells).

Topic to Investigate:
The Morse-Witten model describes the forces acting between bubbles in contact. The force law governing the interactions between bubbles is more complicated than the simple Hooke's law; there is a logarithmic force term and the force acting on a bubble at any contact depends on all the other contacts that this bubble may have.

We have developed software in our group which implements the Morse-Witten model, and thus allows for the simulations of (so far only small) clusters of bubbles. The aims of the project are a further exploration of the code (e.g. bubbles in confined spaces, clusters of bubbles of different sizes), and a further improvement of the visualisation of the computed structures.

Day-to-day nature of the research:
The student will work under the close supervision of one of S. Hutzler's PhD students to assist in the evaluation of the existing code. A love for programming and Python skills are essential for this project. Progress (and lack of progress…) will be discussed at frequent meetings with S. Hutzler and at group meetings.

Learning Outcomes:
- Introduction to open-ended research
- Knowledge of principles of packing problems and soft matter
- Knowledge of advanced programming skills

PROJECT #2: Manufacturing of Berkovich shape diamond nanomechanical AFM probes with micro-moulding technique

Supervisor: Prof. Graham Cross and Dr. Majid Fazeli Jadidi

Research Area: Optimization of nanomechanical characterization methods with Atomic Force Microscopy.

Topic to Investigate:
Atomic Force Microscopy (AFM)-based Nanoindentation, comparing with conventional nanoindentation instruments, offers precise control of the sample deformation in the nanometer range facilitated by accurate force control to obtain local mechanical properties of nano-objects. In addition, conductive diamond probes provide a unique opportunity to investigate nanoelectromechanical properties of piezoelectric and semiconducting nanostructure such as nanowires. Commonly, AFM Nanoindentation market uses a very tedious and expensive method for making diamond Berkovich probes. We are developing an innovative fabrication technique for producing diamond AFM probes with moulded Berkovich tips based on indenting on suitable metal with commercially available Berkovich indenter as a mould to grow diamond Berkovich tip by chemical vapor deposition technique (CVD).

Day-to-day nature of the research:
In this project we will evaluate potential candidate materials such as Chromium, Tungsten, Tantalum as a mould by patterning the metal foil by series of indents with various loads ranging from few mN to 1 N to produce indents with depth of 100s of nanometer up to few microns. After diamond synthesis is done via CVD technique, metal will be preferentially etched from the interface and individual Berkovich shape diamond will be released via different milling techniques which will be mounted on AFM cantilever afterwards (see Figure). This project specifically, will focus on evaluating the candidate metal moulds and optimizing the indentation to obtain desirable Berkovich shape and size. Besides, various type of wet etching process to separate diamond from Chromium, Tungsten or Tantalum with minimum destruction of the tip will be investigated. Subsequently, we will investigate the moulded tips with various imaging techniques such as optical microscopy, SEM, AFM and will study the mechanical characterization of tips with nanoindentation technique.

PROJECT #3 Observations of exocometary CO gas in the beta Pictoris disk with UV Hubble Space Telescope and IR ground-based observations

Supervisor: Prof. Luca Matrà

Research Area:
The majority of nearby, young (10s of million year-old) stars host bright disks/belts of icy exocomets akin to the Kuiper Belt in our Solar System, also known as debris disks. While these were previously thought to be gas-free, Atacama Large Millimeter/submillimeter Array (ALMA) observations now have the sensitivity to detect gas, particularly carbon monoxide (CO), likely released from exocometary ices within the disk. A puzzling ALMA result has been that the excitation temperature of the gas, measured by comparing the amount of light emitted by CO molecules transitioning down between different rotational levels, is as low as <~10 K, suggesting that the CO gas is colder than its freeze-out temperature, just above ~20K. However, this excitation temperature can differ from the true, kinetic temperature of the gas if the molecules are not in thermal equilibrium, and/or because of optical depth effects.

Topic to Investigate:
This project will exploit the potential of combined UV HST and IR ground-based observations of tens of CO rovibronic (UV) and rovibrational (IR) transitions to measure the kinetic temperature separate from excitation temperature and optical depth effects. The CO gas is detected in absorption along the line of sightto the stellar background, as the disk is observed to be edge-on from Earth (see Figs). By simultaneously modelling available observations across the wavelength range, we plan to achieve the most accurate constraints on the abundance of CO along the line of sight, and demonstrate that the CO kinetic temperature is much higher than the excitation temperature as measured by ALMA. In doing so, the aim will be to show that the molecules are not in thermal equilibrium, and the gas is low in density and thus confirm its release by exocomets orbiting the star.

PROJECT #4

Supervisor: Prof. Neale Gibson

Research Area:
Understanding the atmospheres of exoplanet atmospheres. Exoplanets are simply planets that orbit stars other than our Sun. Astronomers have discovered thousands of them in the last few decades, and are currently developing methods to probe their atmospheres.

Topic to Investigate:
This project will use data from the James Webb Space Telescope (JWST) or a large ground-based facility like ESO's Very Large Telescope to extract a spectrum of an exoplanet, allowing us to probe the chemistry and physical properties of the atmosphere.

Day-to-day nature of the research:
This project will focus on data analysis and statistics. The student will spend most of their time writing python code to analyse light curves and/or time-series spectra to extract an exoplanet's spectrum. Depending on the interests of the student, there may also be opportunities to study atmospheric physics and apply modelling techniques to understand the atmosphere.

PROJECT #5: A machine-learning based classifier for extragalactic transients

Supervisor: Prof. Kate Mcguire
Co-Supervisors: Dr. Umut Burgaz/Dr Georgios Dimitriadis

Research Area:

The game-changing Vera C. Rubin Observatory's Legacy Survey of Space and Time (LSST, www.lsst.org) will find hundreds of thousands of extragalactic transients and supernovae when it begins operations in 2024. We aim to use the new multi-object spectrograph 4MOST (www.4most.eu) to take spectra of tens of them a day to rapidly classify the events so that we understand their explosions, their used in cosmology, and their production of heavy elements. For this, an automated classifier is required. A number of classifiers exist but only recently have machine-learning based algorithms been developed (Muthukrishna et al. 2019, Fremling et al. 2021) and they have not been tested for 4MOST.

Topic to Investigate:

In this project, the student will investigate the application of machine-learning based algorithms, e.g. convolutional neural networks to simulated 4MOST spectroscopy. They will also help develop a new training set for the classifier that takes into account the full diversity of current samples. One particularly interesting aspect is the detection of 'outliers' - unknown events that have not been seen in any data previously but that LSST will be capable of detection and may have exciting origins.

Day-to-day nature of the research:

This research is computational in nature with Python the preferred language. The TCD transients research group is diverse and we strive for an friendly and collaborative working environment with weekly group meetings and research discussions.

PROJECT #6 Automating Electron Microscope Control for Atomic-resolution Electric Field Measurement

Supervisor: Prof. Lewys Jones

Research Area:
The scanning transmission electron microscope (STEM) is one of the most sensitive imaging instruments in use in materials research, it can yield magnifications of 40 million times or more and directly image individual atoms within a specimen. In the STEM, by using an electron sensor with four quadrants to measure small deflections of the electron beam, the transmitted electrons can be used to produce differential phase contrast enabling imaging of material's electrostatic potential at atomic resolution [1]. However, such detailed measurements require the electron beam to be precisely centred in the middle of the beam sensor which can be challenging and tedious to realise manually creating a bottleneck in nanomaterials investigations.

Topic to Investigate:
In this project we will design and build a pair of Raspberry Pi controlled motors to automate the x and y beam position knobs. The intensity falling across the four detector quadrants will be read out continuously using existing signal acquisition hardware in the group, and code will be written to automate the instrument alignment. Simulations (Python based) will be used to determine whether the desired results have been realised.

Day-to-day nature of the research:
By the end of the project, we aim to have: 1) Designed, 3d-printed and tested a pair of motor-controlled knobs to augment the hand-panels for the operator, 2) Installed and tested the setup on the electron microscope (student will be supported by other group members), and 3) Tested and demonstrated an improvement in the achieved precision from automatic alignment versus manual attempts. The project and desk space will be based in the Advanced Microscopy Laboratory (www.tcd.ie/crann/aml), for a number of weeks over summer 2023.

References:

[1] Sánchez-Santolino et al., "Probing the Internal Atomic Charge Density Distributions in Real Space", ACS Nano 12, 9, 8875–8881 (2018).

[2] Lin et al., "Analytical transmission electron microscopy for emerging advanced materials", Matter 4, 7 (2021).

PROJECT #7

Supervisor: Prof. Mark Mitchison

Research Area:
Quantum sensing is an emerging technology that harnesses the bizarre features of quantum mechanics to make amazingly precise measurements, e.g. to detect tiny magnetic or gravitational fields. One way to do this is to exploit the extreme sensitivity of a system close to a quantum phase transition, where a dramatic change occurs from one phase to another. Remarkably, quantum phase transitions can occur even in small systems with only a few degrees of freedom, opening the possibility of designing very compact quantum sensors based on this effect.

Topic to Investigate:
The aim of this theoretical project is to design a quantum sensing protocol using a simple model exhibiting a quantum phase transition, known as the Rabi model. The Rabi model describes the interaction of a quantum bit (qubit) coupled to a cavity, which is relevant for a variety of experiments in atomic and mesoscopic physics including modern quantum computing platforms. The student will investigate how interactions with the external environment affect the capability of this quantum Rabi sensor to detect weak external fields.

Day-to-day nature of the research:
This is a theoretical project so the majority of the work will involve analytical (pen and paper) calculations and performing some simple numerical simulations, as well as discussing the underlying physics with the supervisor and other members of the group. Through this project, the student will improve their understanding of quantum mechanics and learn some advanced concepts that are not covered in the Physics undergraduate course. They will also gain experience of scientific computer simulation and improve their programming skills.

PROJECT #8

Supervisor: Prof. Felix Binder and Dr. Marco Radaelli

Research Area: Quantum Information Theory is the area of Theoretical Physics that deals with concepts such as measurements, quantum entanglement and information entropy. The key questions revolve around the idea of *information*, seen as a fundamental physical concept. Within this area, flourishing research is currently happening in the study of quantum random walks.

Topic to investigate. The main topic of investigation will be estimation theory on quantum random walks: how to estimate the value of a parameter encoded in the dynamics of a quantum walker. To do so, AI techniques, such as neural networks, will be employed.

Day-to-day nature of the research. The project is mainly computational (with a possible theoretical perspective if the student is particularly inclined in that direction): the student will code in Python their own engine for simulating a quantum random walk, and then feed the results to a neural network created with Keras. On a day-to-day basis, the student is expected to write and debug code, and discuss and physically interpret the results.

PROJECT #9: Natural Language Process for precise materials data extraction

Supervisor: Prof. Stefano Sanvito

Research Area:
Computational Physics, Machine Learning, Artificial Intelligence

Topic to Investigate:
Natural Language Processing (NPL) is branch of artificial intelligence that aims at making written and spoken language interpretable by a machine. Most of the research is concentrated on what is called sentiments analysis, namely in categorising text according to some classes (e.g. identify what a text is about). A much less charted territory concerns the extraction of precise information from a text. In this project we will investigate how to represent a text into a mathematical form (representation), which then can be handled by machine learning. The final objective is to automatically extract physical information concerning materials from scientific articles.

Day-to-day nature of the research:
1. Learn the basics of machine learning and in particular of natural language processing.
2. Collect a dataset of texts including the desired information (crystallographic data, critical temperatures)
3. Evaluate different relation classification strategies to resolve conflicts related to multiple information.
4. Construct a number of machine-learning model for data extraction.

Python familiarity is required.

PROJECT #10

Supervisor: Prof. Stephen Dooley

Research Area:
Machine learning studies of the chemical physics of carbon dioxide electrochemical reduction.

Topic to Investigate:
Energy sciences by numerical modelling studies of complex chemical physics, molecular thermodynamics and reaction kinetics.

Day-to-day nature of the research:
Desk based studies, working from home or from laboratory. Numerical simulation by exercising and developing the MLOCK (Machine Learned Optimisation of Chemical Kinetics) in-house written code. Competence or interest in learning of python, matlab or other math orientated data processing package for multiple linear regressions & principal component analyses, machine learning toolkits (tensorflow, splunk, pytorch), physics based chemical physics modelling through density functional theory (Gaussian, GAMES) and device orientated physics solvers (cantera, chemkin, comsol).

PROJECT #11

Supervisor: Prof. Stephen Dooley

Research Area:
Machine learning studies of the chemical physics of hydrogen in advanced gas turbine combustion.

Topic to Investigate:
Energy sciences by numerical modelling studies of complex chemical physics, molecular thermodynamics and reaction kinetics.

Day-to-day nature of the research:
Desk based studies, working from home or from laboratory. Numerical simulation by exercising and developing the MLOCK (Machine Learned Optimisation of Chemical Kinetics) in-house written code. Competence or interest in learning of python, matlab or other math orientated data processing package for multiple linear regressions & principal component analyses, machine learning toolkits (tensorflow, splunk, pytorch), physics based chemical physics modelling through (cantera, chemkin, comsol)

PROJECT #12

Supervisor: Prof. Stephen Dooley

Research Area:
Machine learning studies of the sustainable aviation fuel certification properties – relating electronic structure theory to fluid property measurement.

Topic to Investigate:
Energy sciences by numerical modelling studies of complex chemical physics, molecular thermodynamics and reaction kinetics.

Day-to-day nature of the research:
Desk based studies, working from home or from laboratory. Numerical simulation by exercising and developing the MLOCK (Machine Learned Optimisation of Chemical Kinetics) in-house written code. Competence or interest in learning of python, matlab or other math orientated data processing package for multiple linear regressions & principal component analyses, machine learning toolkits (tensorflow, splunk, pytorch), physics based chemical physics modelling through (cantera, chemkin, comsol)

PROJECT #13: Spin decoherence in molecular qubits

Supervisor: Prof. Alessandro Lunghi

Research Area:
Quantum physics, computational physics, magnetic properties

Topic to Investigate:
In recent years, quantum science has evolved from a fundamental theory used to explain physical phenomena, to an active player in modern technologies. The spin of electrons behaves as a prototypical 2-level quantum system and therefore represents the ideal quantum bit (qubit), i.e. the logical unit of a quantum machine. In this project the student will use state-of-the-art quantum mechanical calculations to describe the time evolution of the quantum states associated with the spin of a magnetic molecule, namely a molecular qubit.

Day-to-day nature of the research:
The project is computational in nature. The student will use the Python library PyCCE to efficiently simulate the evolution of the spin state of a series of magnetic molecules. The intern will also develop Python script to analyze and interpret the results obtained with PyCCE. The student will regularly meet with the supervisor and will take part to the supervisor's group activities, such as group meetings and seminars.