Trinity College School of Physics Summer Undergraduate Research Experience 2022

PROJECT #1: The statistics of small boat motion

Supervisor: Prof. Stefan Hutzler

Research Area:

The rescuing of migrants on board of often very small vessels in the Mediterranean requires knowledge of their precise location. Unlike commercial and also many private boats, these vessels are generally not equipped with an automated identification signaling system which would allow for their tracking (AIS data). Space Eye(*), a non-profit organisation made up of scientists and students with a mainly data-science background, aims to use instead freely available satellite data to assist in determining vessel location.

Topic to Investigate:

Satellite data is of limited spatial and temporal resolution. The location of a vessel some time after such a snapshot can thus only be predicted. This requires knowledge of the characteristics of the vessel motion, which is likely to feature significant drift, due to the large impact of local wind and water movements on a small boat.

Day-to-day nature of the research:

The project concerns a statistical analysis of the motion of boats using ASI data. This data bank provides also information on the size of each tracked vessel, current speed etc. The aim is to correlate velocity fluctuations with vessel characteristics. Knowledge about the drift statistics of small boats may ultimately be used to make predictions about the locations of refugee vessels.

The student will interact with S. Hutzler and his PhD students on a regular basis. Data sets will be provided by Space Eye, who will also participate in some of the project meetings.

Learning Outcomes:

- Expertise with using large data sets
- Knowledge of tools of basic statistical analysis

PROJECT #2: Experimental studies of sphere packings

Supervisor: Prof. Stefan Hutzler

Research Area:

Arrangements of spheres in confinement, buckling, instabilities, bifurcations

Topic to Investigate:

A linear chain of spheres, confined in a transverse harmonic potential, is unstable and buckles under compression or tilt. The student will perform experiments involving a number of realizations of this phenomenon, e.g. ball bearings in a cylinder or gas bubbles in a water filled cylinder, which might also be rotating, using a lathe.

Day-to-day nature of the research:

The student will work under the guidance of a PhD student in an experimental lab, with regular interaction with S. Hutzler and his group.

Learning Outcomes:

- Skill in designing and evaluating an experiment
- Knowledge of simple image analysis, data processing, and data presentation

Supervisor: Prof. Brian Espey

Research Area:

Light pollution and energy use

Topic to Investigate:

The research proposed is an application of a new geo-based technique developed by Prof. Espey to combine digital elevation (LiDAR) data, council lighting databases and lighting photometry to study area- and city-wide light emission to determine the influences on the city emission function, i.e. how much light is emitted in which direction. This information is necessary in order to determine the energy budget of light pollution, the impact of light on the wider environment, and the total lighting energy budget of a city using International Space Station data and satellite-based measurement

Day-to-day nature of the research:

The program will use freeware R and QGIS geographic information systems (GIS) packages which are powerful tools used in geographical-based approaches, though R also has powerful statistical applications, including in astrophysics. After the introductory period, a typical day will involve the generation of theoretical model outputs for a range of typical urban environments and their comparison with quantitative imaging obtained from space to determine the accuracy of the models. Learning outcomes will include the facility for fluent use of the GIS packages and an understanding of the importance and quantification of light pollution as a form of energy loss which will be of use to local authorities. It is hoped that the project will lead to a publication.

PROJECT #4: Exploring the diversity of Type Ia supernova environments

Supervisor: Prof. Kate Mcguire and Dr. Umut Burgaz

Research Area:

This project will focus on improving our understanding of the origin of Type Ia supernovae, the explosive deaths of white dwarfs in binary systems. Type Ia supernovae are vital for understanding the cosmological make-up of the Universe but we don't yet understand how they explode. However, clues to their origin can be obtained from the types of galaxy environments in which they explode (e.g. old versus young stellar populations, metallicity).

Topic to Investigate:

In this project, the student will investigate the environmental properties of a large sample of Type Ia supernovae obtained with the state-of-the-art transient detection survey, the Zwicky Transient Facility. They will use machine-learning techniques to identify outliers in the sample that can be used to constrain Type Ia supernova explosion mechanisms. These outliers will then be compared to theoretical predictions with the aim of obtaining cleaner samples for future cosmological measurements.

Day-to-day nature of the research:

This research is computational in nature with Python the preferred language. The student will make use of machine-learning packages such as scikit-learn. The TCD transients research group is diverse and we strive for an friendly and collaborative working environment.

PROJECT #5: Constraining light curve 'kinks' in Type Ia supernovae

Supervisor: Prof. Kate Mcguire and Dr. Georgios Dimitriadis

Research Area:

Type Ia supernovae are used in cosmology to determine distances in the universe because they behave like standard candles. However, progress in the quality and quantity of telescope observations have uncovered unexpected irregularities in the light curves of Type Ia supernovae. This could have important consequences for using them in cosmological studies.

Topic to Investigate:

This project will investigate and characterise the newly discovered "kink" in the light curves (Pessi et al. 2021) by analysing data from the Zwicky Transient Facility, a leading transient discovery and follow-up survey. The origin of these 'kinks' remains unclear but is likely related to the properties of the white dwarf (e.g. density, composition) at the time of explosion that in turn affects the temperature and structure of the ejecta.

Day-to-day nature of the research:

This project is purely computational, requiring the student to work at a desk (or at home). During the first few weeks, the student will need to become accustomed with handling large databases. Once the student has a grasp of the data set, data analysis techniques written in Python will be implemented to study the light curves, and machine learning techniques could be harnessed to investigate whether the "kink" in the light curves is predictive of other Type Ia supernovae properties.

Supervisor: Prof. Lewys Jones

Research Area:

This project relates to the high-resolution transmission electron microscopes (TEMs) based in the Advanced Microscopy Lab, part of the CRANN centre in TCD. The TEM focusses electrons using intense magnetic fields generated by wire coils carrying large currents (up to 3,000 amp-turns in some lenses). These lenses produce heat through resistive heating and must be cooled 24/7 to maintain a fixed resistance and performance.

Topic to Investigate:

This project will involve the audit, modelling and analysis of the heat produced, the heat flows, and the heat sinks in the TEM cooling system. The goal is to investigate if some (or all) of the >500W of heat output can be met by sustainable cooling technologies. We hope that this will lead to a reduction in both electricity use and carbon-footprint for the overall system.

Day-to-day nature of the research:

The student will work in the Ultramicroscopy group alongside PhD students and a post-doc to assess the existing heat loads and the current water cooling system on the TEM. Over the summer we will design and build a new piping system to utilise passive cooling to the outside air, possibly night-time thermal reservoirs, and potentially to explore the use of ground-source heat systems. We would hope to end the summer with a quantitative estimate of the reduction in energy/carbon achieved, and to prepare a report to document the findings potentially for academic publication.

PROJECT #7: Optical computing with polariton condensates

Supervisor: Prof. Paul Eastham

Research Area:

This research area involves understanding the quantum mechanical behaviour of light interacting with electrons in solids. It can explore fundamental questions, such as the nature of quantum coherence and the emergence of order from many-particle states, and is also relevant for applications. The work typically involves building theories rooted in the Schroedinger equation, and using them to study how light and matter interact, predict the consequences of those interactions, and relate those predictions to experiments.

Topic to Investigate:

The proposed topic is optical computing with polariton condensates. These are forms of Bose-Einstein condensate formed from quasiparticles in semiconductors, which display fascinating properties, including macroscopic quantum coherence. They have been used to produce proof-of-principle demonstrations of a type of optical computer for solving physics problems, and you would explore theoretically how useful such a device would be if it is applied to real problems.

Day-to-day nature of the research:

The research would be based on our recent paper on synchronization of coupled oscillators, and your goal would be to apply this framework to the polariton-based optical computer. This would entail reading papers and doing pen-and-paper analytical work, developing and analyzing models of the problem, as well as some computation in Mathematica or Python. You would join the Quantum Theory of Light and Matter Group, and be able to chat to PhD students in that group, and potentially also discuss this work electronically with our collaborators in the U.K. and U.S.

Supervisor: Prof. Mark Mitchison

Research Area:

One of the most fascinating discoveries in physics in the last few decades is the existence of topological phases of matter. These materials have remarkable and bizarre properties: they are completely robust to local perturbations and they may support fractional quasi-particles, i.e. emergent excitations of a many-electron system that carry only a fraction of the electron's charge. Understanding the behaviour of these systems, both in and out of equilibrium, is among the foremost challenges of modern quantum physics research.

Topic to Investigate:

In this theoretical physics project we will investigate a new scheme for testing whether a many-body system is in a topological phase. The idea is to introduce a small quantum system – in this case, a single two-level spin or qubit – that probes the many-body system. We create a quantum superposition of the two qubit states and observe how it evolves in time under the influence of its surroundings – the dynamics should be very different depending on whether the system is topological or not.

Day-to-day nature of the research:

The research will involve a mixture of analytical theory calculations and numerical simulations of a concrete model. The student will have a chance to develop their own code, perform exploratory numerical experiments, and try to understand the physics with the help of Prof. Mitchison – a successful project could even lead to a publication. The project would suit a student who enjoys computer programming and would like to get a better understanding of one of the most peculiar and beautiful areas of quantum physics.

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

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 text representations against data extraction.

4. Construct a number of machine-learning model for data extraction

Familiarity with Python is required

PROJECT #10: Natural Language Process for topic identification

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). In this project we will explore how NPL sentiment analysis can work to identify the paragraph within a scientific article that discusses about a target property. This will operate on a corpus of scientific papers extracted from literature.

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. Construct a number of machine-learning models for topic identification.

4. Run the model against published paper and construct an enlarged dataset for further refinement.

Python familiarity is required.

PROJECT #11:

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 (cantera, chemkin, comsol)

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)

Supervisor: Prof. Stephen Dooley

Research Area:

Machine learning studies of the sustainable aviation fuel certification properties – relating chemical structure to fluid property.

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 #14: Unsupervised learning of magnetic ions' chemical space

Supervisor: Prof. Alessandro Lunghi

Research Area:

machine learning, computational physics, magnetic properties

Topic to Investigate:

The computational designing of new compounds is one of the new frontiers of materials science. In recent years, machine learning has made it possible to predict materials properties based on the sole knowledge of their chemical structure and composition, therefore bypassing the need of synthesizing a large number of compounds before individuating the optimal one for a given application. In this project, the student will generate a data set of magnetic compounds with different chemical structures and will apply unsupervised machine learning algorithms in order to predict the configurations with optimal properties for magnetism and quantum technology applications.

Day-to-day nature of the research:

The project is computational in nature. The student will learn the basics of machine learning and how to code simple models for the analysis of small data sets. The student will use Python scripting together with state-of-the-art machine learning libraries such as TensorFlow or Pytorch. The student will take part to the supervisor's group activities, such as group meetings and seminars and will be supervised by Prof Lunghi and the postgraduate student Ms Nguyen.

Learning outcomes:

- Understanding of algorithms for unsupervised learning of data sets
- Development of familiarity with crystallographic databases

PROJECT #15: Electronic structure of solid-state spin qubits

Supervisor: Prof. Alessandro Lunghi and Dr Sourav Mondal

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 electronic structure and magnetic properties of solid-state defects, such as NV centers in diamond, which have been proposed as optimal candidates for quantum-technology applications. This study will shine light on how to optimize new materials in order to further improve spin qubits properties for specific applications.

Day-to-day nature of the research:

The project is computational in nature. The student will learn the basics of electronic structure theory and how to run quantum mechanical calculations. The student will use python scripting for manipulating data as well as state-of-the-art software for quantum mechanical calculations, such as Orca and Cp2k. The student will take part to the supervisor's group activities, such as group meetings and seminars, and will be co-supervised by the research fellow Dr Mondal, who will guide the student in the use of high-performance computing facilities and electronic structure codes.

Learning outcomes:

- Understanding of electronic structure methods
- Understanding of spin qubits functionality