

Quantum non-linear transformations and “Third Quantization”

Supervisor: Andrew Mitchell [andrew.mitchell@ucd.ie]

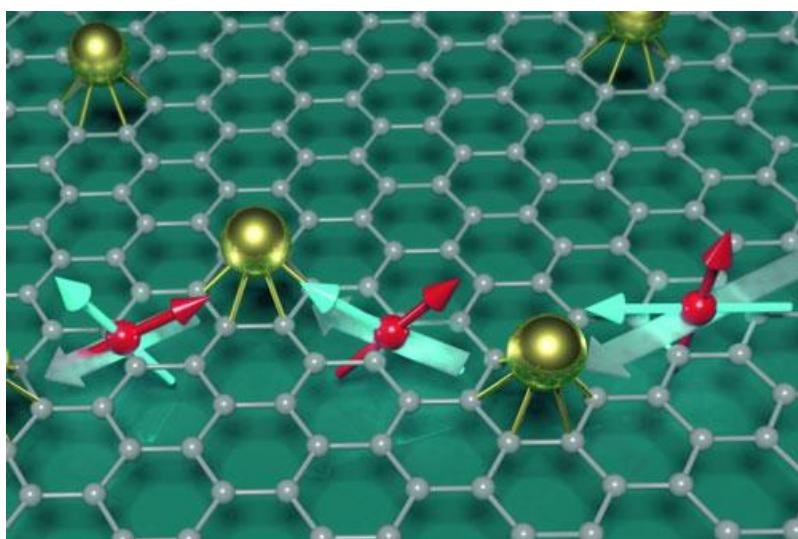
Theme: Quantum

Quantum condensed matter physics describes real mesoscopic or macroscopic systems in terms of the collective properties of their many interacting quantum constituents. Examples of mesoscopic systems include nanoelectronic devices, currently being developed as new quantum technologies; while macroscopic quantum systems include materials such as superconductors and graphene.

A cornerstone of many-particle quantum mechanics is “second quantization” – an efficient and elegant formulation of the theory in which quantum properties are encoded in the algebra of operators that act to generate arbitrary states from the vacuum. The Schrodinger Equation is solved by a basis transformation in the space of many-particle states. Conventionally, this transformation is linear, often being expressed in the language of matrix transformations. However, it has recently been shown that a new set of non-linear transformations exist, based on a decomposition in terms of fractionalized “Majorana” fermions. But what are the consequences of these transformations? Do they provide a new route to solving hard quantum problems? Is there a connection to another recent theory – “third quantization”, which involves superoperators working in commutator space?

This project will explore these conceptually new ideas in the context of simple quantum models. It will involve learning quantum many-body physics, second quantization, tight-binding formalism, Green’s function methods, and coding in Mathematica.

This is a theoretical project that will involve both analytical calculations and numerical simulations.



References:

- [1] Bruus & Flensberg. “*Many-body quantum theory in condensed matter physics.*” OUP textbook, 2004.
- [2] “In Search of Majorana...” <https://www.nature.com/articles/nphys3275>
- [3] “Majorana Returns!” <https://www.nature.com/articles/nphys1380>

System-Environment decoherence and non-Hermitian Hamiltonians

Supervisor: Andrew Mitchell [andrew.mitchell@ucd.ie]

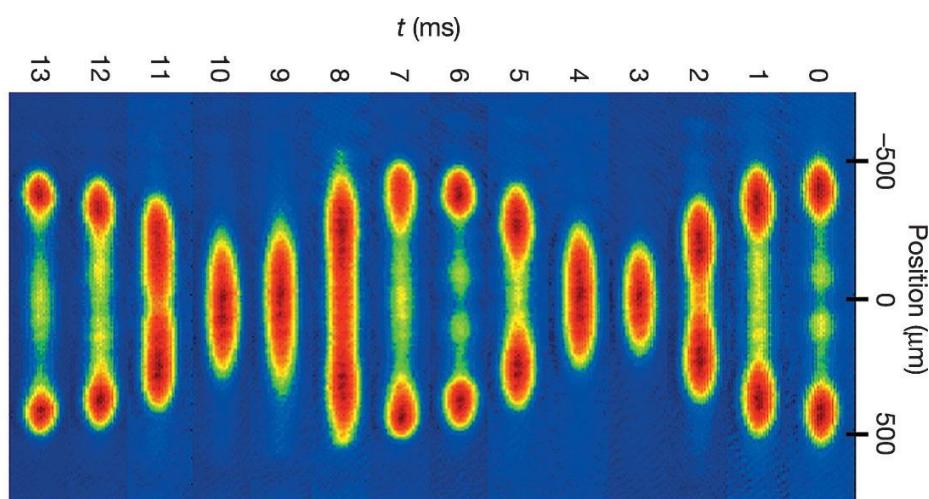
Theme: Quantum

The standard lore in quantum theory is that the Hamiltonian of a system should be Hermitian. This guarantees that the Hamiltonian eigenvalues (energies) are real numbers, as required for a physical observable. However, this concept has recently been challenged, with non-Hermitian Hamiltonians now being used as effective models of open quantum systems. The imaginary part of complex ‘energies’ in such systems is interpreted as a scattering rate induced by a decohering environment. Furthermore, certain non-Hermitian Hamiltonians do have pure real eigenvalues (energies) – but now the eigenvectors (wavefunctions) are not orthogonal. This can be interpreted as quantum mechanics with a deformed metric for the underlying Hilbert space. What does this mean?!

In this project you will explore these conceptually new ideas and look at Hermitian quantum systems coupled to explicit quantum environments to derive effective non-Hermitian models for the ‘open’ quantum system with an implicit environment.

The project will involve learning quantum many-body physics, second quantization, tight-binding formalism, Green’s function methods, and coding in Mathematica.

This is a theoretical project that will involve both analytical calculations and numerical simulations.



References:

- [1] Bruus & Flensberg. “*Many-body quantum theory in condensed matter physics.*” OUP textbook, 2004.
- [2] “*Making sense of non-Hermitian Hamiltonians*”, Bender. Reports on Progress in Physics (2007)
<https://iopscience.iop.org/article/10.1088/0034-4885/70/6/R03/>
- [3] “*Non-Hermitian physics*”, El-Ganainy et al. Nature Physics (2018)
<https://www.nature.com/articles/nphys4323>

Thermodynamics of coherent quantum control

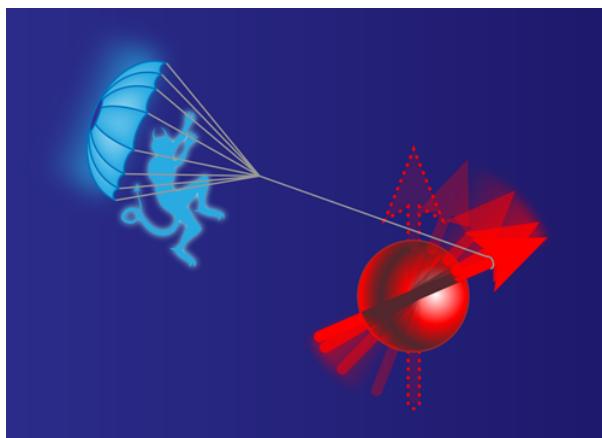
Supervisor: Steve Campbell [steve.campbell@ucd.ie]

Theme: Quantum

To achieve the full promise of next generation quantum technologies, not only must we be able to manipulate the fragile quantum states, but we must also carefully assess the thermodynamic cost of achieving this control. Indeed, a quantum device that requires exponential resources will never be truly viable. Recently, significant effort has been invested into designing protocols that allow for perfect control of quantum systems on, in principle, arbitrarily short timescales. However, the development of the theory of quantum thermodynamics has since demonstrated that these techniques can come at a high thermodynamic and complexity cost in terms of the excess energy required to achieve this control.

In this project we will critically examine the thermodynamics of several commonly used control protocols. Focus will be given to examining the work statistics of the controlled dynamics, looking beyond averages to higher order moments of the full work distribution and how this relates to the complexity of the applied protocol.

This is a theoretical project that will involve both analytical and numerical simulations.



References:

- *Shortcuts to adiabaticity: Concepts, methods, and applications*
D. Guéry-Odelin, A. Ruschhaupt, A. Kiely, E. Torrontegui, S. Martínez-Garaot, and J. G. Muga
Rev. Mod. Phys. **91**, 045001 (2019)
<https://journals.aps.org/rmp/abstract/10.1103/RevModPhys.91.045001>
- *Energetic cost of quantum control protocols*
O. Abah, R. Puebla, A. Kiely, G. De Chiara, M. Paternostro, and S. Campbell
New J. Phys. **21** 103048 (2019)
<https://iopscience.iop.org/article/10.1088/1367-2630/ab4c8c/meta>
- *The role of quantum work statistics in many-body physics*
J. Goold, F. Plastina, A. Gambassi, and A. Silva
arXiv:1804.02805
<https://arxiv.org/abs/1804.02805>

Multipartite non-locality in distributed quantum registers

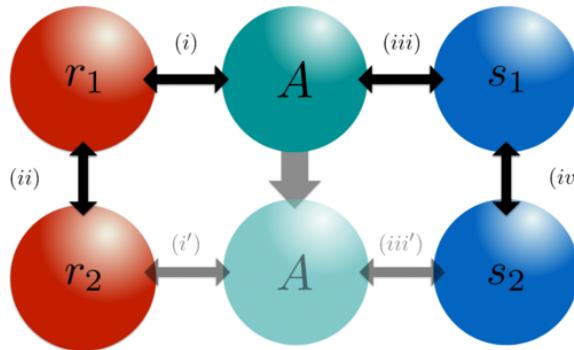
Supervisor: Steve Campbell [steve.campbell@ucd.ie]

Theme: Quantum

A remarkable aspect of quantum mechanics is its inherently non-local nature, i.e. the curious fact that for quantum systems comprised of two or more constituents that have interacted (imagine for instance two electrons that collided at some point) the act of measuring one of these electrons affects the state of the other, even if they are separated by vast distances. This concept can be made mathematically rigorous for the simplest case of two qubits, leading to the famous Bell inequality. Characterising the correlations in a such bipartite systems is fairly easy: two subsystems are either correlated or not. For multipartite quantum systems the situation is significantly more involved.

In this project we will examine whether and how quantum correlations are established within and across two quantum registers. Employing multipartite extensions of Bell's theorem, the correlation strength and structure will be probed and we will examine how the microscopic description of the interactions plays a role.

This is a theoretical project that will involve both analytical and numerical simulations.



References:

- *Detecting Genuine Multipartite Quantum Nonlocality: A Simple Approach and Generalization to Arbitrary Dimensions*
Jean-Daniel Bancal, Nicolas Brunner, Nicolas Gisin, and Yeong-Cherng Liang
Phys. Rev. Lett. 106, 020405 (2011)
<https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.106.020405>
- *Robust multipartite entanglement generation via a collision model*
Barış Çakmak, Steve Campbell, Bassano Vacchini, Özgür E. Müstecaplıoğlu, and Mauro Paternostro
Phys. Rev. A 99, 012319 (2019)
<https://journals.aps.org/pra/abstract/10.1103/PhysRevA.99.012319>
- *Multipartite nonlocality in a thermalized Ising spin chain*
Steve Campbell and Mauro Paternostro
Phys. Rev. A 82, 042324 (2010)
<https://journals.aps.org/pra/abstract/10.1103/PhysRevA.82.042324>
- Experimental linear-optics simulation of multipartite non-locality in the ground state of a quantum Ising ring
Adeline Orieux, Joelle Boutari, Marco Barbieri, Mauro Paternostro, and Paolo Mataloni
Sci. Rep. 4, 7184 (2014)
<https://www.nature.com/articles/srep07184>

Fast and robust control in double quantum dots

Principal Supervisor: Anthony Kiely [anthony.kiely@ucd.ie]

Co-Supervisor: Steve Campbell [steve.campbell@ucd.ie]

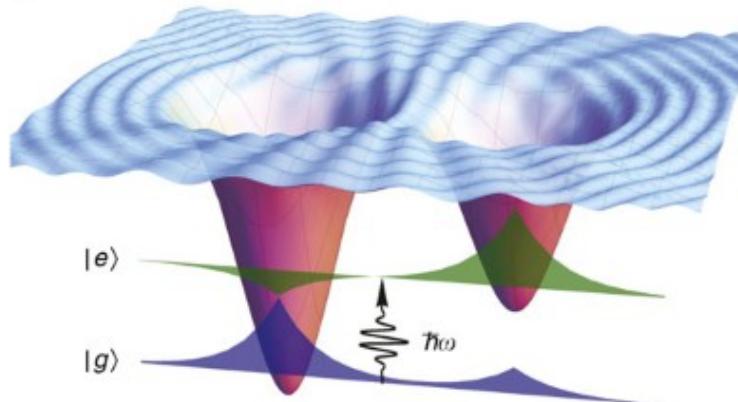
Theme: Quantum

Fast control of complex quantum systems is an important step to fully realise future quantum technologies. Previously effective control has been achieved using adiabatic methods, however these require long operation times leaving the system exposed to the detrimental effects of environment (decoherence).

For the specific case of the double quantum dot, fast high fidelity control can be achieved [1] using the methods inverse engineering. However reformulating this in terms of Lewis-Riesenfeld invariants [2] would allow for a simpler parameterisation of the control fields, which in turn could be used to counteract experimental imperfections [3].

In this project we will design control fields using Lewis-Riesenfeld invariants and use this in combination with perturbation theory to combat different errors such as spin dependent tunnelling rates and population leakage [4].

This is a theoretical project that will involve both analytical and numerical work.



References:

- [1] Yi-Chao Li et. al., New J. Phys. 20 113029 (2018)
- [2] D. Guéry-Odelin et. al., Rev. Mod. Phys. 91, 045001 (2019)
- [3] A. Kiely and A. Ruschhaupt, J. Phys. B: At. Mol. Opt. Phys. 47 115501 (2014)
- [4] X. Li et. al., Phys. Rev. A 96, 012309 (2017)

Shockwave induced bubble collapse, microjets and their manipulation with nanomaterials

Supervisor: Donal MacKernan [Donal.MacKernan@ucd.ie]

Theme: complex fluids and advanced nano-materials

Cavitation is a dynamic process in which a bubble occurs, grows, and collapses inside or on the liquid– solid interface when the local pressure of a liquid is reduced to its saturated vapor pressure. It can be induced in various ways, including the action of propellers, the application of lasers or intense ultrasound and shock-waves. The shock waves and liquid jets that can accompany bubble collapse can damage materials, but can also be used in medicine when suitably focused. In the context of advanced materials it can be used to break up carbon nanotube bundles or the exfoliate graphene sheets.

The objective of the present theoretical physics project is to explore how the presence of nano-materials like carbon nanotubes and graphene in liquids such as water facilitate cavitation and the formation of nano-jets. Advanced simulation using super computers make such an exploration feasible using methods that include computational fluid dynamics, mesoscale simulation, molecular dynamics and hybrid combinations thereof. The project will therefore involve the use of statistical mechanics, fluid and molecular dynamics, coding e.g. use of python or C++, and super-computers. The project will be structured so as to first reproduce recent published works and the step by step to explore open problems. As a research project, the applicant(s) will be expected to show considerable self-initiative but be able to benefit from the support of a team when needed.

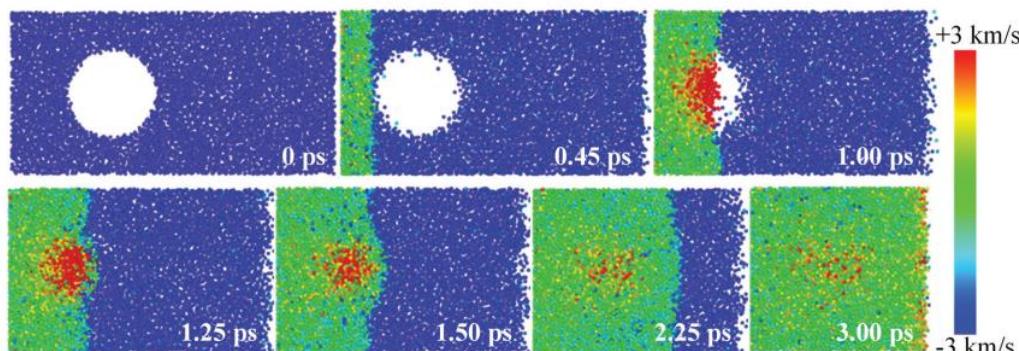


Fig. 1 Sequence of snapshots of the shock wave propagation through the water for $D = 5.0$ nm at $u = 3.0$ km/s see reference [1]

References:

- [1] S. Zhan et al, “**Shockwave induced bubble collapse, microjets and their manipulation with nanomaterials**”, Phys. Chem. Chem. Phys., 23, 8446, 2021
- [2] Colin Denniston et al, “**LAMMPS lb/fluid fix version 2: Improved hydrodynamic forces implemented into LAMMPS through a lattice-Boltzmann fluid**”, Computer Physics Communications, 2022
- [3] C. Peng et al “**Simulation of multiple cavitation bubbles interaction with single-component multiphase Lattice Boltzmann method**”, International Journal of Heat and Mass Transfer, Volume 137, July 2019, Pages 301-317.
- [4] Jonas Latt et al, “**Palabos: Parallel Lattice Boltzmann Solver**”, Computers & Mathematics with Applications, Volume 81, 2021

Designing microfluidic devices using computational fluid dynamics and molecular dynamics

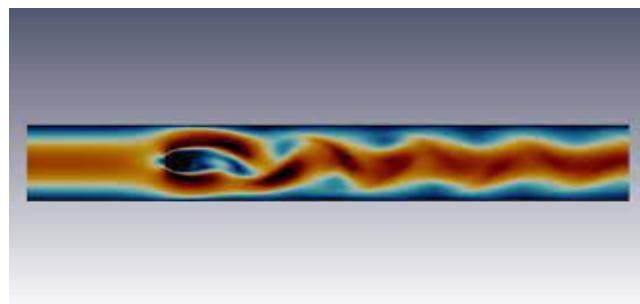
Supervisor: Donal MacKernan [Donal.MacKernan@ucd.ie]

Theme: complex fluids, molecular transport and surface interactions

The miniaturization of many technologies to sub-micron scales ranging from electronics to medical devices is an ongoing scientific and industrial revolution with concomitant challenges and opportunities. For example, multiphase fluids, such as droplets and bubbles, are commonly found in such applications, and surface effects, especially surface wettability, become significant due to the large surface-to-volume ratio, and sensitive to the choice and morphology of device materials. Advanced simulation methods and super-computers are increasingly used to test and validate blueprints before anything is actually made.

The objective of the present theoretical physics project is to design microfluidic chambers and interconnection conduits suitable for the performance of bio-assays including the transport and detection of viruses. The project will involve the use of statistical mechanics, the [Lattice Boltzmann Method](#) (LBM), mesoscale and molecular dynamics running on super-computers, and some coding using of python or C++. As a research project, the applicant(s) will be expected to show self-initiative but be able to benefit from the support of a team when needed.

Fig. 1 Velocity flow field of a fluid in a narrow pipe simulated with the Lattice Boltzmann method using



Palabos[1]

References:

[1] Jonas Latt et al, “Palabos: Parallel Lattice Boltzmann Solver”, Computers & Mathematics with Applications, Volume 81 (2021)

[2] Colin Denniston et al, “LAMMPS lb/fluid fix version 2: Improved hydrodynamic forces implemented into LAMMPS through a lattice-Boltzmann fluid”, Computer Physics Communications (2022).

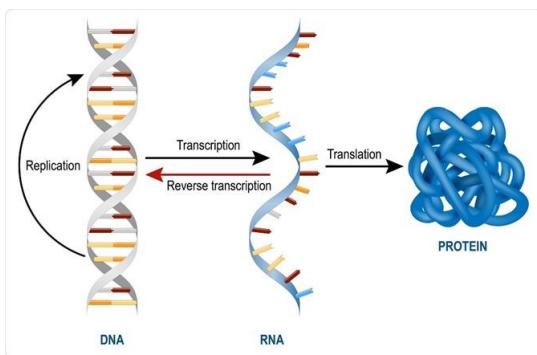
Controlling the Structure and Dynamics of mRNA

Supervisor: Donal MacKernan [Donal.MacKernan@ucd.ie]

Theme: Biophysics

At the basis of life is the genetic code of DNA, its transcription into single helical mRNA, and translation into protein. Transcription and translation are molecular processes, where in each case a large molecular formed by a sequence of nucleic acids provides the blueprint for the building of another molecule. DNA and RNA are each formed by 4 nucleic acids, and proteins are formed by amino acids, of which 20 are used biologically. A triplet of nucleic acids defines a codon, and the simple observation that there are 64 possible codons might suggest that there is some form of degeneracy where more than one codon can give rise to the same amino acid, that is codons are synonymous. In fact, in each genome, synonymous codons for the same amino acid are used with different frequencies; this general phenomenon is known as codon bias. It turns out that this bias is not purely accidental, but can have a major effect on the successful translation of mRNA into protein. Recently the UCD School of Physics has developed a platform technology consisting of protein based molecular switches which are synthesized using genetic engineering at the UCD Conway Institute of Molecular Biology and Medicine. An important step in the process of synthesis is the choice of synonymous codon sequence in suitable hosts. The main focus of this theoretical physics project is the exploration of the structural and dynamical properties of mRNA using advanced simulation, deep learning, so as to optimize protein expression.

The project will therefore involve the use of statistical mechanics, molecular and mesoscale dynamics, deep learning, coding e.g. use of python, and super-computers. As a research project, the applicant(s) will be expected to show self-initiative but be able to benefit from the support of a team when needed.



References:

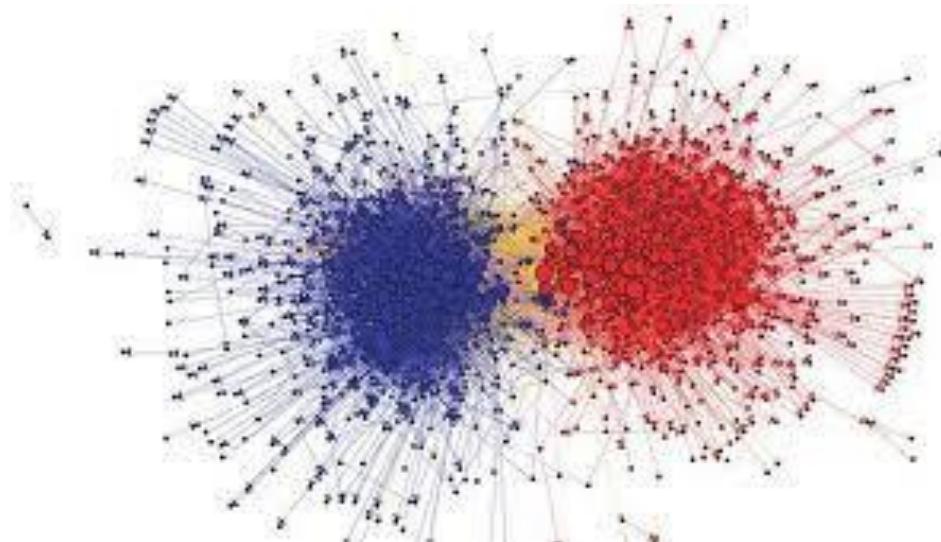
- [1] Davide Arella et al “Codon usage bias and environmental adaptation in microbial organisms”, Molecular Genetics and Genomics (2021) 296:751–762
- [2] Hongguang Fu et al, “Codon optimization with deep learning to enhance protein expression”, Scientific Reports, (2020) 10:17617
- [3] Bikash K. Bhandari et al, “Analysis of 11,430 recombinant protein production experiments reveals that protein yield is tunable by synonymous codon changes of translation initiation sites”, PLoS Comput Biol 17(10) (2021)
- [4] Jiri Sponer et al, “RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview”, Chemical Reviews 2018 118 (8), 4177-4338
- [5] Donal MacKernan, “Molecular Sensors”, US Patent 16/331327

“Physics of collective behavior”

Supervisor: Vladimir Lobaskin [vladimir.lobaskin@ucd.ie]
Theme: Statistical physics / social physics

While it is impossible to predict a behaviour of a person or an animal using only basic physics laws, motion of a large crowd or a flock can often be predicted quite accurately. Large scales make details and motives of individual behaviour unimportant, while the symmetry of motion and interactions play the central role. In this project, you will learn about mechanisms of dynamic self-organisation in systems of active agents, about standard models of collective behaviour, and apply methods of non-equilibrium statistical physics to study of opinion dynamics or flocking.

Applications to recent social and political movements (COVID, Brexit, BLM) may be considered. This is a theoretical project that will involve numerical simulations.



Recent publications on the topic:

1. Romensky, M., Spaiser, V., Ihle, T., Lobaskin, V. Polarized Ukraine 2014: opinion and territorial split demonstrated with the bounded confidence XY model, parametrized by Twitter data. R. Soc. Open Sci. 2018, <http://doi.org/10.1098/rsos.171935>
2. M. Romensky, V. Lobaskin, T. Ihle, Tricritical points in a Vicsek model of self-propelled particles with bounded confidence, Phys. Rev. E 90, 063315 (2014)
3. M. Romensky, D. Scholz, V. Lobaskin, Hysteretic dynamics of active particles in a periodic orienting field, J. R. Soc. Interface 12, 20150015 (2015)

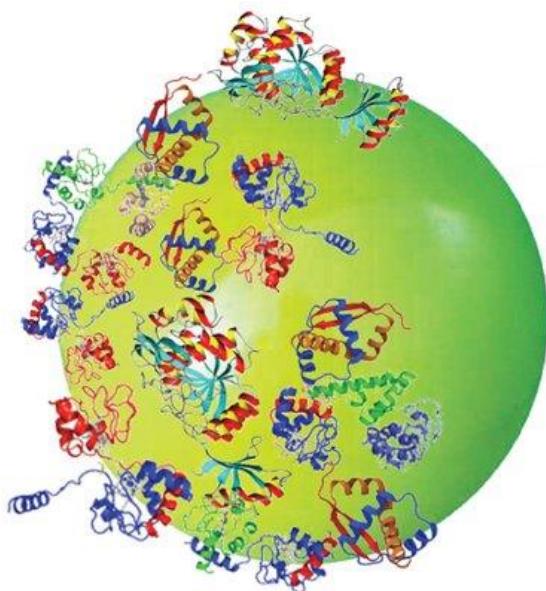
“Computational modelling of bio-nano interactions”

Supervisor: Vladimir Lobaskin [vladimir.lobaskin@ucd.ie]

Theme: Nano-bio physics

Nanoparticles and nanowires are currently used in various applications ranging from cosmetics, medicine and food to electronics and smart materials. Due to large surface-to-volume ratios they may be extremely active and sometimes harmful to living organisms. We are trying to understand the molecular mechanisms of bio-nano interactions and predict nanoparticle activity in biological environments. We use multiscale models including molecular modelling, condensed matter theory and machine learning to construct models of nanoparticle protein corona. The specific applications include toxicity screening or design of drug delivery engines. The project will combine molecular modelling and machine learning methods to construct a competitive adsorption model and predict the protein corona and binding of antibodies to nanoparticles.

This is a theoretical project that will involve numerical simulations.



Recent publications on the topic:

1. I. Rouse, D. Power, E. G. Brandt, M. Schneemilch, K. Kotsis, N. Quirke, A. P. Lyubartsev, V. Lobaskin, First principles characterisation of bio-nano interface, *Phys. Chem. Chem. Phys.* 2021, 23, 13473-1348261.
2. Alsharif, S.A.; Power, D.; Rouse, I.; Lobaskin, V. In Silico Prediction of Protein Adsorption Energy on Titanium Dioxide and Gold Nanoparticles. *Nanomaterials* 2020, 10, 1967.
3. Power D, Rouse I, Poggio S, Brandt E, Lopez H, Lyubartsev A, Lobaskin V. A multiscale model of protein adsorption on a nanoparticle surface, *Modelling Simul. Materials Sci. Eng.* 27:084003 (2019)

Super-luminous Supernovae

Supervisors: Morgan Fraser [morgan.fraser@ucd.ie]

Peter Duffy [peter.duffy@ucd.ie]

Theme: Astrophysics

Core-collapse supernova arise from the explosion of a massive star at the end of its life. They release on the order of 10^{44} J of energy, making them some of the most energetic phenomena in the universe. Supernova are also a key site for explosive nucleosynthesis, and are responsible for seeding the cosmos with heavy elements.

Supernovae are fiendishly complex, and detailed computational simulations typically include radiation transport, magnetohydrodynamics, GR effects, nuclear reactions and more (and require millions of CPU-hours to run). However, one can also gain considerable insight into supernovae through simple one-dimensional semi-analytic models (Arnett 1982).

In this project, you will construct a simple semi-analytic model for a supernova and apply it to help understand the class of "super-luminous supernovae". To begin, we will assume a homologously expanding explosion, powered by the decay of radioactive ^{56}Ni in its centre. Over the course of the project, you will further develop this model by exploring different power sources; specifically you will replace ^{56}Ni with the energy deposited from a rapidly rotating, highly magnetic neutron star (Kasen & Bildsten 2010) and examine the impact of these effects on the explosion's hydrodynamics. Such a model has been suggested to explain bright super-luminous supernovae which are too energetic to be powered solely by the decay of radioactive ^{56}Ni (Inserra et al. 2013).

This project will require the student to be comfortable with solving differential equations that describe the evolution of a supernova, as well as coding in Python. In addition to the core TP modules, students should also have taken optional modules in Astronomy and enrol for the Theoretical Astrophysics module.

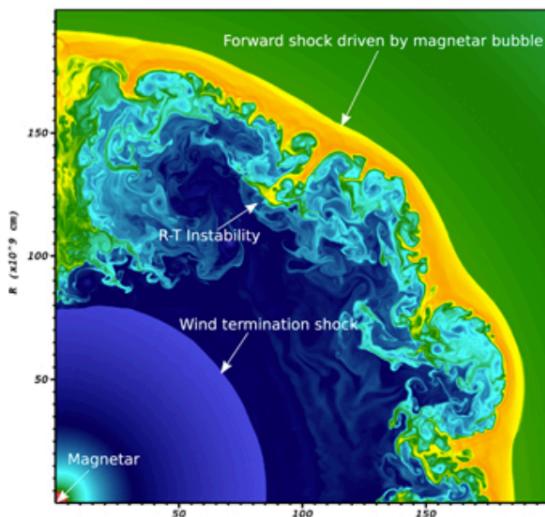


Figure : A 2D slice through a detailed hydrodynamic model of a superluminous supernova explosion (Chen et al 2016). Colours indicate density in the ejecta.

References:

Arnett (1982) <https://articles.adsabs.harvard.edu/pdf/1982ApJ...253..785A>

Kasen & Bildsten (2010) <https://iopscience.iop.org/article/10.1088/0004-637X/717/1/245/pdf>

Inserra et al. (2013) <https://iopscience.iop.org/article/10.1088/0004-637X/770/2/128/pdf>

4th-year Research Project

Quasi-Normal Modes of Black Holes

Supervisor: Prof Adrian Ottewill

Motivation

It was noted four decades ago that a perturbed black hole will, after an initial response, emit radiation with well-defined frequencies and rates of damping, in the manner of a bell sounding its last dying pure notes. These damped resonances, called Quasinormal modes (QNMs), play a key role in black hole dynamics. Mathematically, ‘quasinormal ringing’ emerges from a sum of residues of poles of the Green function in the complex frequency domain with each pole corresponds to a QNM of a single (complex) frequency. The real part of the (complex) frequency corresponds to the oscillation rate and the (negative) imaginary part corresponds to the damping rate.

In a spherically symmetric space-time (such as the Schwarzschild space-time), the QNM frequencies ω_{ln} are labelled by two integers: multipole l and overtone $n \geq 0$. The properties of the QNM spectrum depends only on the properties of the field (e.g. spin) and the black hole geometry (e.g. mass, charge, angular momentum).

The high-overtone spectrum has a beautiful and ornate structure, which has inspired speculation that highly-damped QNMs may be linked to, e.g., Hawking radiation, black hole entropy, or loop quantum gravity. QNMs are also of relevance to holographic principles such as the AdS/CFT conjecture.

The Project

In spinning black hole space-times a key step is to determine the (spin-weighted) spheroidal harmonics, a generalization of spherical harmonics which however are frequency-dependent. In a recent paper Vickers and Cook [arXiv:2208.06259v1](https://arxiv.org/abs/2208.06259v1) discovered unexpected behaviour of the spheroidal harmonics for complex frequencies, in particular, for large complex frequencies related to highly damped overtones.

This project may be taken in two directions:

- *Numerical*: Write code in Mathematica to validate Vickers and Cook’s using confluent Heun functions rather than numerical spectral methods.
- *Analytical*: Obtain an analytical understanding using the methods of Casals, Ottewill & Warburton in [arXiv:1810.00432](https://arxiv.org/abs/1810.00432).

Note: Students must be taking ACM40750 General Relativity and Black Holes to undertake this project.

4th-year Research Project

Hawking Radiation

Supervisor: Prof Adrian Ottewill

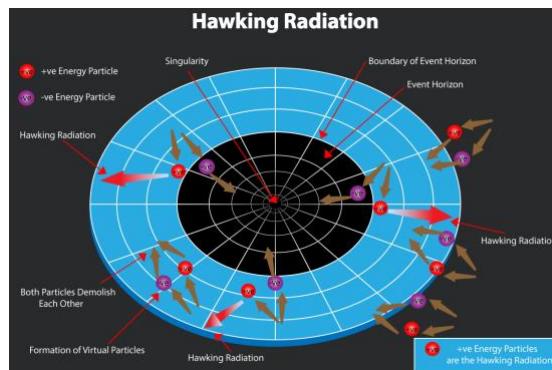
Motivation

Black holes are one of the most interesting objects that have emerged from Einstein's General theory of Relativity. They are defined as regions of spacetime where spacetime itself is so distorted that not even light can escape from them; this is what makes them appear "black".

However, Stephen Hawking realised early on that black holes have a temperature and entropy associated with their event horizon and they obey the laws of thermodynamics, much like a pot of boiling water. Exploring these ideas further using quantum mechanics, in 1975 he shocked the physics world by arguing that black holes are not quite black, but instead glow slightly by emitting radiation. This radiation is known as "Hawking radiation". In this project you will learn about the first and second law of black hole thermodynamics, and you will study Hawking radiation.

Classically, by taking the Fourier transform, a field may be thought of as an infinite collection of harmonic oscillators. On quantization each of these harmonic oscillators acquires zero-point energy so the quantum vacuum is filled with oscillations.

In this project you will explore how this zero-point energy can be effected by static 'mirrors', the so-called Casimir effect, by moving mirrors, and its relation to the so-called Unruh effect. Finally, you will see how the gravitational redshift arising a star collapsing to a black holes has the same effect as the Doppler redshift of a receding mirror leading to vacuum energy being converted into radiated particles that make up Hawking radiation.



References:

- Hawking, S. W. (1975). "Particle creation by black holes". Communications in Mathematical Physics. 43 (3): 199–220. doi:10.1007/BF02345020.
- Lecture notes on Black Holes by Fay Dowker.

Note: Students must be taking ACM40750 General Relativity and Black Holes to undertake this project.

Visualisation of an accretion disk around a Schwarzschild black hole as seen by infalling observers

Sarp Akcay

The film *Interstellar* features the most realistic visualisations of a spinning black hole-accretion disk system. This project will take the first steps toward this visualisation by constructing the projected image of a thin accretion disk around a non-spinning (Schwarzschild) black hole as seen by in-falling observers. The student will first learn about the Schwarzschild spacetime and null (lightlike), timelike geodesic orbits. The student will then solve the geodesic ODEs and build trajectories of light-beams in the equatorial plane. The next step will be to construct the images of an infinitely thin accretion disk as seen by a fixed equatorial observer, then to extend the previous techniques to build snapshots of the accretion disk as seen by an observer radially falling into the black hole from a generic direction in three dimensional space. This final step can further be generalized to include inspiralling observers. Ideally, the work should also take into account the gravitational redshifting of the color of the accretion disk.

The project will require the student to know/learn some general relativity and working knowledge of solving differential equations. The computational work can be done using **Mathematica**/Python/C(++) . It is recommended that the student do the preliminary work with **Mathematica** then move onto the Python/C(++) for the “production” runs. The figure below shows a snapshot of the target image.

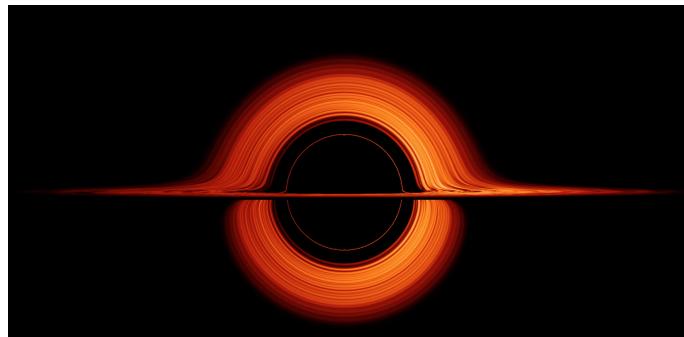


Figure 1: An infinitely thin accretion disk around a Schwarzschild black hole as seen from a position above the equatorial plane. Image courtesy of NASA Goddard Space Flight Center.

Estimating the Parameters of Gravitational Wave Sources

Sarp Akcay and Niels Warburton

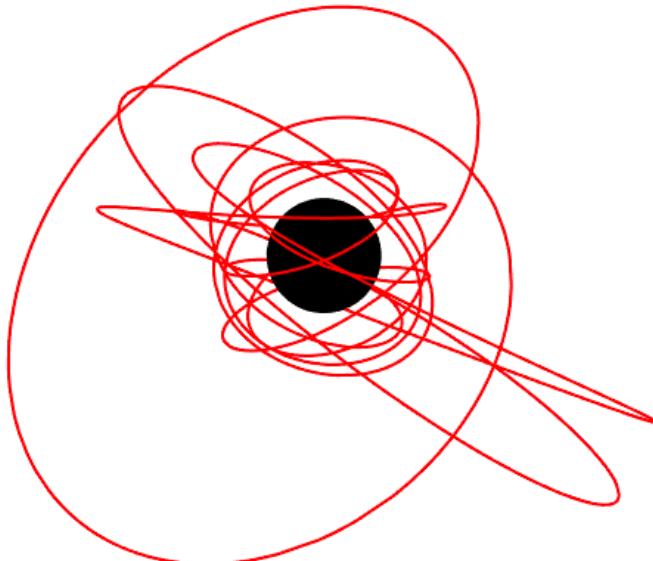
Detection of gravitational waves has now become routine with roughly 100 sources to date. However, a gravitational-wave signal alone does not tell us anything about the source(s) emitting it. Source parameters are obtained through a lengthy process involving data analysis (e.g. detector noise characterisation) and parameter estimation. Scientists employ theoretical gravitational-wave models to construct what an incoming wave may look like at a given detector. The imprint of the wave further depends on the so-called extrinsic parameters such as distance and sky position. Parameter estimation essentially takes a given theoretical wave, subtracts it from the detector data, and looks at whether or not the remainder is “innocuous” noise. The theoretical foundation of parameter estimation is Bayesian statistics and the computations are performed using Markov chain Monte Carlo methods on large-scale computing clusters.

The aim of this project is to build a gravitational wave parameter estimation “from scratch”. We will start by constructing a likelihood function from the Fourier transforms of Newtonian (quadrupole) waveforms against flat and coloured Gaussian noise backgrounds. We will then conduct simple one and two dimensional injection-recovery studies to see how the likelihood behaves over a small patch of the parameter space. Using reasonable, but also adequately agnostic prior, we will construct posterior distributions using our likelihood. We will then generalize these techniques to more realistic waveforms with more parameters. Finally, we will attempt our own parameter estimation studies of synthetic gravitational wave signals using Markov Chain Monte Carlo approaches to walk through the parameter space.

Orbital motion about a black hole

Supervisor: Niels Warburton [niels.warburton@ucd.ie]
Theme: General Relativity and Black Holes

When a compact object, such as a neutron star or stellar mass black hole, strays too close to a massive black hole it will be ensnared by its gravitational pull. Initially, the orbital trajectory will be large Newtonian-like ellipses. Over time the binary will emit gravitational waves which will shrink the orbit. Just as Einstein demonstrated that his theory of general relativity caused Mercury's perihelion to precess about the Sun, the compact object's orbit will start to precess. For orbits around a black hole this precession is taken to the extreme, leading to 'zoom-whirl' orbits [1] which can precess by an arbitrarily large amount. If the black hole is a rotating the orbit can also precess about the equatorial plane. These effects led to an extremely complicated and rich structure for orbits about a rotating black hole with an example shown below:



During this project you will study geodesic orbital motion about a rotating black hole learning about the constants of motion, orbital frequencies, precession rates, zoom-whirl orbits and the inner-most stable orbit (the last stable orbit before the body plunges into the black hole). There also is scope to extend this project to explore:

- Trajectories that cross the event horizon and even escape to another universe.
- Capture trajectories that may destroy the black hole's event horizon via overcharging [2].
- The evolution of the binary and the emitted gravitational wave radiation [3]

References:

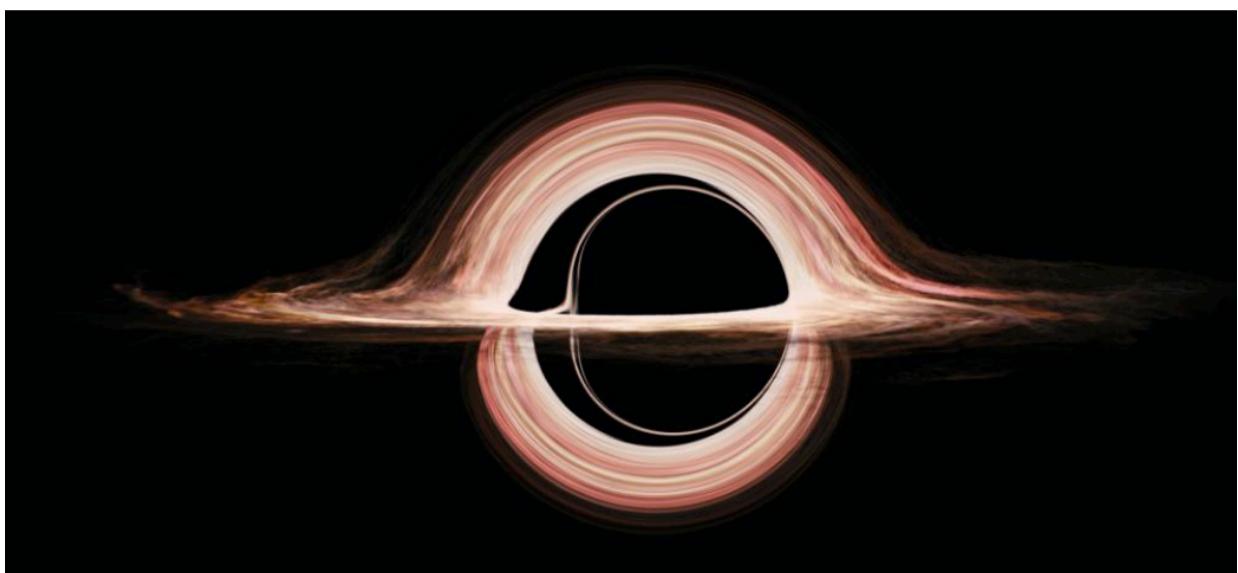
- [1] K. Glampedakis, D. Kennefick, Phys.Rev. D66 (2002), [arXiv:gr-qc/0203086](https://arxiv.org/abs/gr-qc/0203086)
- [2] V. Hubeny Phys. Rev. D 59, 064013 (1999), [arXiv:gr-qc/9808043](https://arxiv.org/abs/gr-qc/9808043)
- [3] C. Cutler, D. Kennefick, E. Poisson, [Phys. Rev. D 50, 3816 \(1994\)](https://doi.org/10.1103/PhysRevD.50.3816)

Black Hole Shadows

Supervisor: Niels Warburton [niels.warburton@ucd.ie]
Theme: General Relativity and Black Holes

The recent direct observation of the massive black hole at the heart of M87 with the event horizon telescope was a breakthrough moment in physics. A key aspect of the analysis was the calculation of the black hole shadow -- the observed region where photons are captured by the black hole.

In this project you will study the motion of light rays that are emitted from a distant source and which eventually reach the position of an observer (or camera), perhaps having passed near the black hole along the way. In practice the light rays are traced backwards in time, starting at the camera, along null geodesics of the black hole metric [1]. Each pixel on the camera image corresponds to a light ray with a different initial momentum vector, which will, as a result, follow a different trajectory; some rays will reach a distant light source, and some will not, having fallen instead behind the event horizon.



One outcome of this project will be a calculation that can render how any picture looks with a black hole in front of it — see above for an advanced version of this. If time allows it can be extended in the following ways:

- to visualise at rotating black holes [2].
- to visualise at wormholes [3].
- visualising simple accretion disk models.
- visualising the light intensity.

References:

[1] The Null Geodesics of the Kerr Exterior, S. E. Gralla, A. Lupsasca, *Phys.Rev.D* 101 (2020), [arXiv:1910.12881](https://arxiv.org/abs/1910.12881)

[2] Gravitational Lensing by Spinning Black Holes in Astrophysics, and in the Movie Interstellar, O. James, E. Von Tunzelmann, P. Franklin, K. S. Thorne, *Am.J.Phys.* 83 (2015), [arXiv:1502.03808](https://arxiv.org/abs/1502.03808)

[3] Visualizing Interstellar's Wormhole, O. James, E. Von Tunzelmann, P. Franklin, K. S. Thorne, *Am.J.Phys.* 83 (2015), [arXiv:1502.03809](https://arxiv.org/abs/1502.03809)

Waveforms from Extreme Mass Ratio Inspirals

Supervisor: Dr Barry Wardell <barry.wardell@ucd.ie>

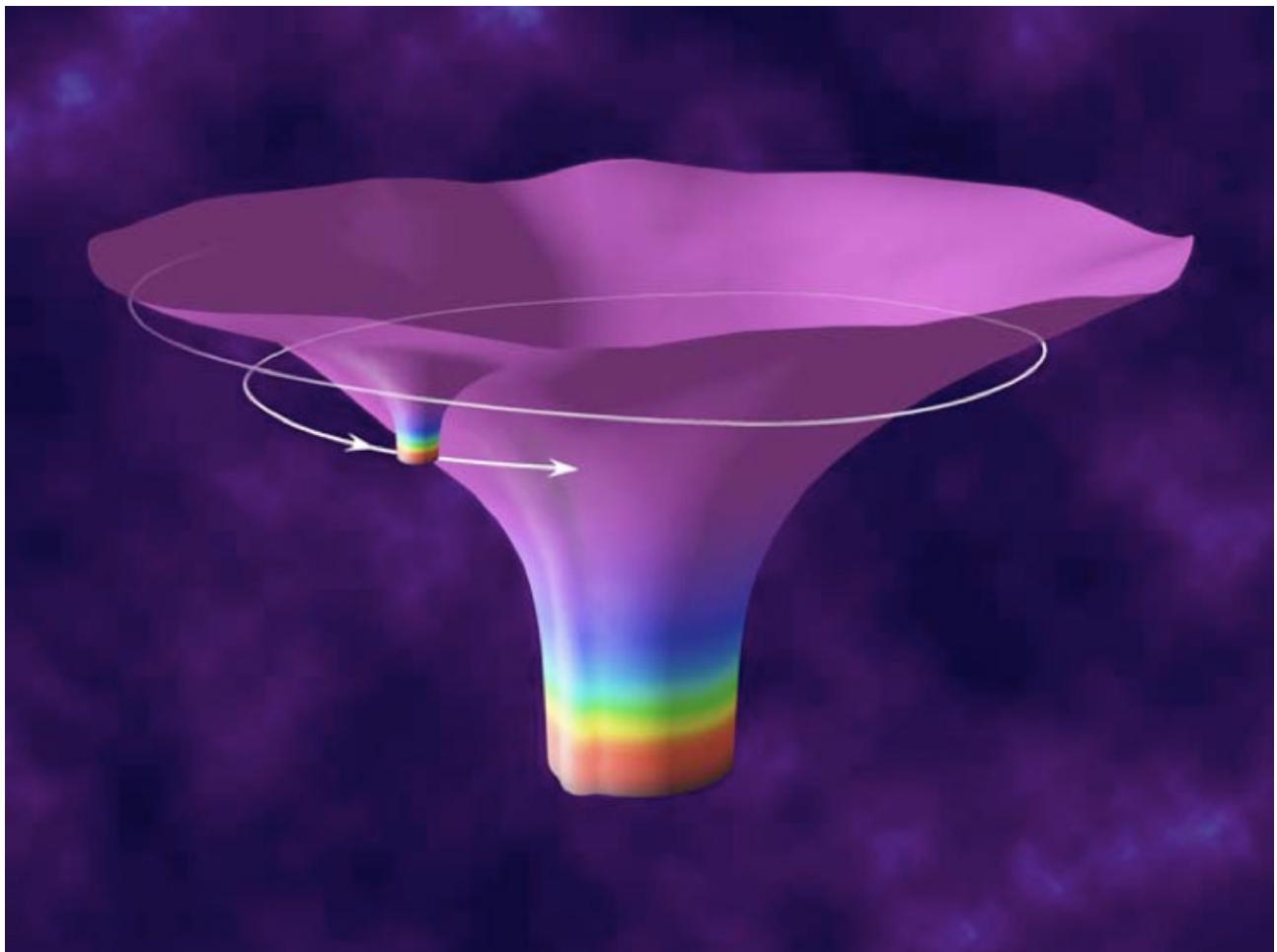
Theme: Black holes and gravitational waves

The breakthrough detection of **Gravitational Waves** by the **LIGO/Virgo Collaboration** (LVC) is generating waves of excitement within the physics community. The detection itself led to the award of the 2017 Nobel Prize in Physics. Even more exciting is that the first detection was only the start. The LVC continues to make groundbreaking discoveries as the detector is tuned to be sensitive to ever more distant sources.

The next quantum leap in GW science will come with the launch of the **Laser Interferometer Space Antenna** (LISA), funded as a flagship European Space Agency L-class mission, and with substantial support from NASA. Just as X-ray, gamma-ray and radio observations of the electromagnetic universe unveiled a host of sources which were previously undetectable by optical telescopes, the sensitivity of LISA to an entirely new GW frequency band will open the field up to a whole new realm of sources such as **extreme mass ratio inspirals** (EMRIs), supermassive binaries, and exotic objects such as cosmic strings.

The LVC demonstrated that a hybrid approach is essential for GW science: experimentalists built the detector, while theoreticians produced models for the expected waveforms from GW sources. These waveforms form a crucial part of the data analysis pipeline; a matched-filtering approach is used to extract signals from noisy GW observations, and this process fundamentally relies on access to accurate waveform models. Without the models, many GW signals would go entirely undetected, and even those that are detected would be poorly understood.

In this project you will study and develop models for the gravitational wave signal from EMRIs based on an adiabatic approximation to the Einstein field equations and making use of black hole perturbation theory.



Numerical Simulations of Binary Black Hole Mergers

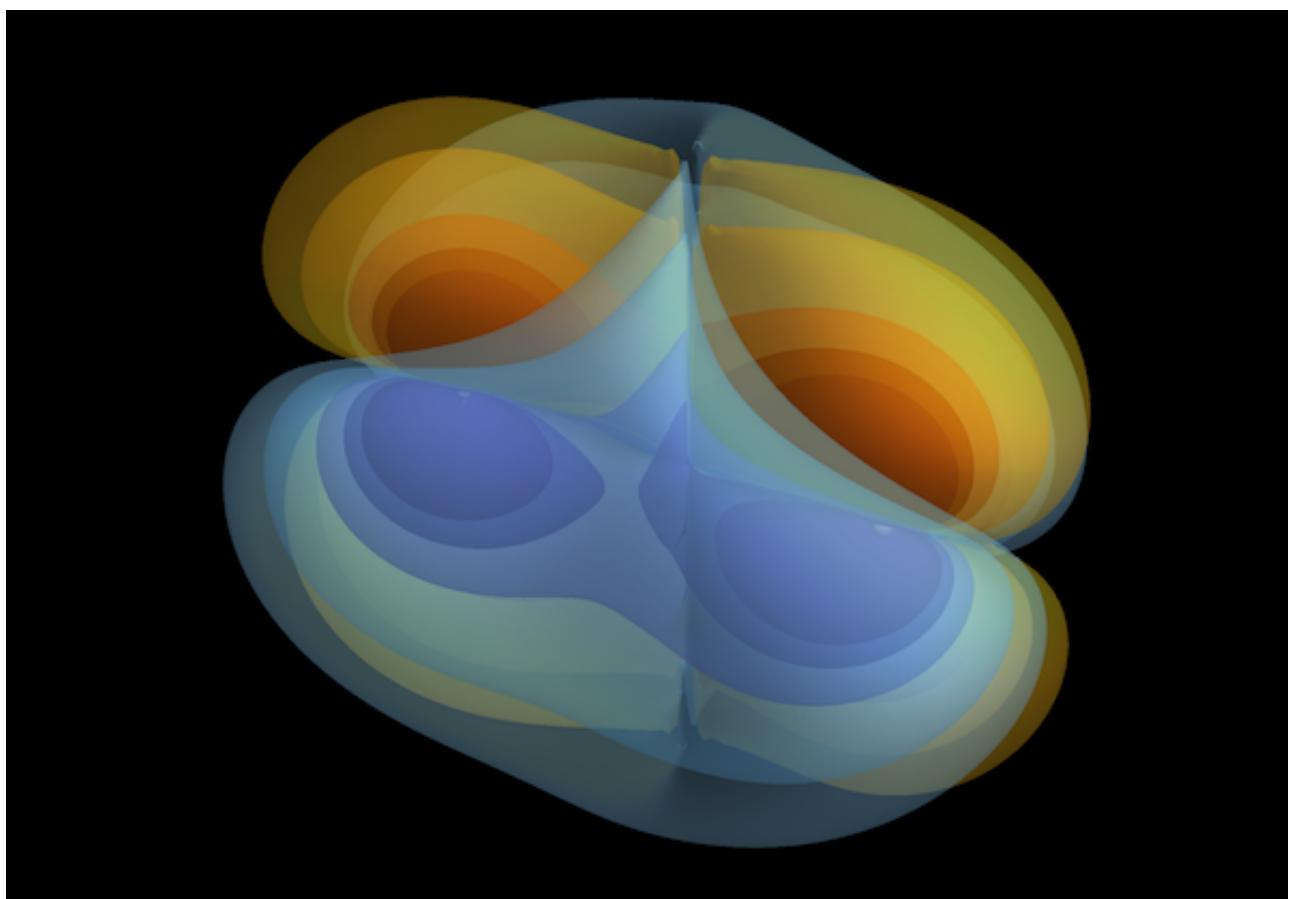
Supervisor: Dr Barry Wardell <barry.wardell@ucd.ie>

Theme: Numerical simulations, black holes and gravitational waves

The Einstein field equations of General Relativity are a nonlinear system of ten coupled partial differential equations for the ten components of the metric tensor describing the spacetime geometry. Physically relevant solutions are notoriously hard to obtain, except in scenarios with a high degree of symmetry. A celebrated example is the Kerr solution, which describes the exterior spacetime of an isolated rotating black hole. But put two such black holes in a bound binary, and their strikingly complex nonlinear interaction again becomes extremely hard to model, even approximately.

One solution to this problem is to use computer simulations to directly solve the Einstein field equations. This use of “Numerical Relativity” to model binary black hole systems has a long and rich history, starting in the early days of scientific computing in the 1970s, through the funding by the US National Science Foundation of the binary black hole Grand Challenge in the 1990s, to the current day where Numerical Relativity simulations play a major role in the study of black holes and neutron stars observed by the LIGO-Virgo-Kagra collaboration.

In this highly computational project you will make use of the Einstein Toolkit <<https://www.einsteintoolkit.org>> open source software to run numerical relativity simulations of the inspiral and merger of a binary black hole system.



Title: Estimating physical and hydrodynamic parameters of cliff-top mega boulder transport using wave-tank experiments

Supervisor: James Herterich (james.herterich@ucd.ie)

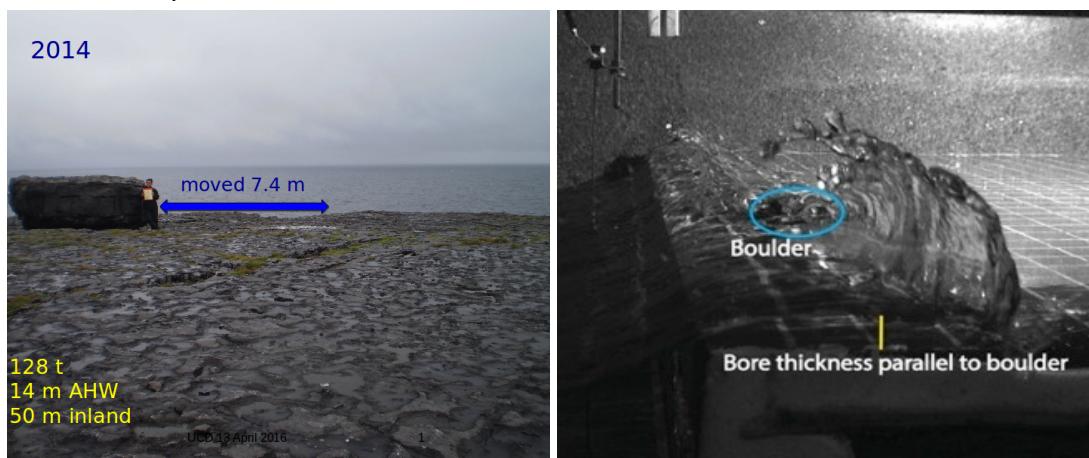
Keywords: Mathematical modelling, geophysical fluid dynamics, parameter fitting, sensitivity analysis

Abstract:

Storm waves impact and overtop coastal platforms in high-energy events. In the most extreme cases, 100+ tonne mega boulders are fractured from bedrock and transported across the platform. Hydrodynamic models capture the physics of the problem. However, there is large uncertainty in parameter values such as coefficients of drag, lift, and inertia, the static and dynamic frictions, and even local fluid speed and acceleration during fluid–structure interaction.

Field observations typically supply a start and end point of transport. While efforts for in-situ measurements are in progress, a set of wave-tank experiments capture a lab-scale version of the problem, including type of impact and details of motion.

The aim of the project is to take numerical simulations of boulder transport (with a working program supplied) and determine appropriate physical and hydrodynamic parameters to fit a dataset of experimental measurements.



References:

Kennedy, Andrew B., et al. "Observations and modeling of coastal boulder transport and loading during Super Typhoon Haiyan." *Coastal Engineering Journal* 58.01 (2016): 1640004.

Cox, Rónadh, Louise O'Boyle, and Jacob Cytrynbaum. "Imbricated coastal boulder deposits are formed by storm waves, and can preserve a long-term storminess record." *Scientific reports* 9.1 (2019): 1-12.

Cox, Rónadh, et al. "Systematic review shows that work done by storm waves can be misinterpreted as tsunami-related because commonly used hydrodynamic equations are flawed." *Frontiers in Marine Science* 7 (2020): 4.

Title: Transformation of sea-bottom pressure measurements to free-surface wave height

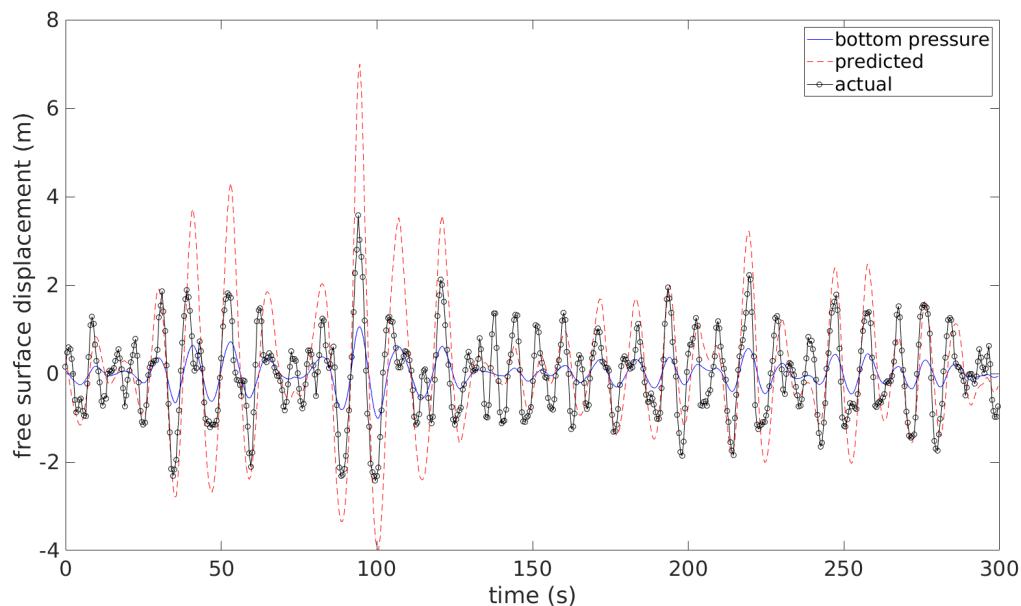
Supervisor: James Herterich (james.herterich@ucd.ie) and Frederic Dias

Keywords: Mathematical modelling, oceanography

Abstract:

Measuring the sea surface is an engineering challenge, especially in rough conditions. A sea bottom-mounted pressure device captures characteristics of the motion of free surface waves. However, wave effects attenuate exponentially with depth even for linear waves. In rougher conditions, nonlinear effects on the free surface are dampened at the bottom. There are a number of models - incorporating more and different physical effects - for transforming sea-bottom pressure measurements to free-surface wave height.

The aim of this project is to compare a number of such models using measurements of bottom pressure and free-surface height. Data is provided from the field experiments off the coast of Inis Meain in 2017.



References:

Vasan, Vishal, et al. "A method to recover water-wave profiles from pressure measurements." *Wave Motion* 75 (2017): 25-35.

Henry, David, and Gareth P. Thomas. "Prediction of the free-surface elevation for rotational water waves using the recovery of pressure at the bed." *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* 376.2111 (2018): 20170102.