UCD Physics
Summer Research Studentships
2024

Project 1. Development of liver lesion surrogates based on patient lesion segmentation, modelling and 3d printing techniques, for image quality assessment in Computed Tomography

Assist. Prof. Irene Hernández-Girón

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Image quality in Computed Tomography (CT) is frequently assessed with test objects (phantoms) mimicking simple geometries (such as cylinders) containing series of patterns to evaluate. The image quality metrics that are traditionally evaluated are noise, contrast, spatial resolution, low contrast resolution...Such phantoms and tests, though they help to characterize some technical aspects of image quality do not represent the attenuation, tissue texture or disease stage present in patients[1]. As CT systems evolve, in particular with iterative and deep- learning based reconstruction (which is usually designed considering that the object imaged is a human body) there is a need for anthropomorphic test objects to evaluate image quality. 3D printed has become a popular manufacturing method to develop such anthropomorphic phantoms, for example for CT lung imaging[2].

In this project, public patient databases will be researched to identify and collect a selection of abdominal cases (liver imaging) containing lesions with different shapes and characteristics[3]. These lesions will be segmented (using freeware such as imageJ[4] and 3D slicer[5]) and transformed into models that will be compatible with 3D printing techniques (Meshmixer, Meshlab software[6]) and a library of lesions will be generated, varying their shape, size and other characteristics. Additionally simple geometries will also be designed for the liver lesions (3D ellipsoids, ovoids...)

Finally, a selection of the lesions of the generated digital library will be manufactured using 3D printing techniques. The lesions will be scanned in an abdominal phantom for CT clinical protocols and images evaluated and compared with patient and commercial anthropomorphic phantom data[7].

References

[1] Verdun et al. Image quality in CT: From physical measurements to model observers. Physica Medica 2015;31:823-843

[2] Hernandez-Giron I, den Harder JM, Streekstra GJ, Geleijns J, Veldkamp WJH. Development of a 3D printed anthropomorphic lung phantom for image quality assessment in CT. Physic Medica 2019 3https://www.cancerimagingarchive.net/access-data/

[4] https://imagej.nih.gov/ij/

[5] https://www.slicer.org/

[6] https://meshmixer.com/

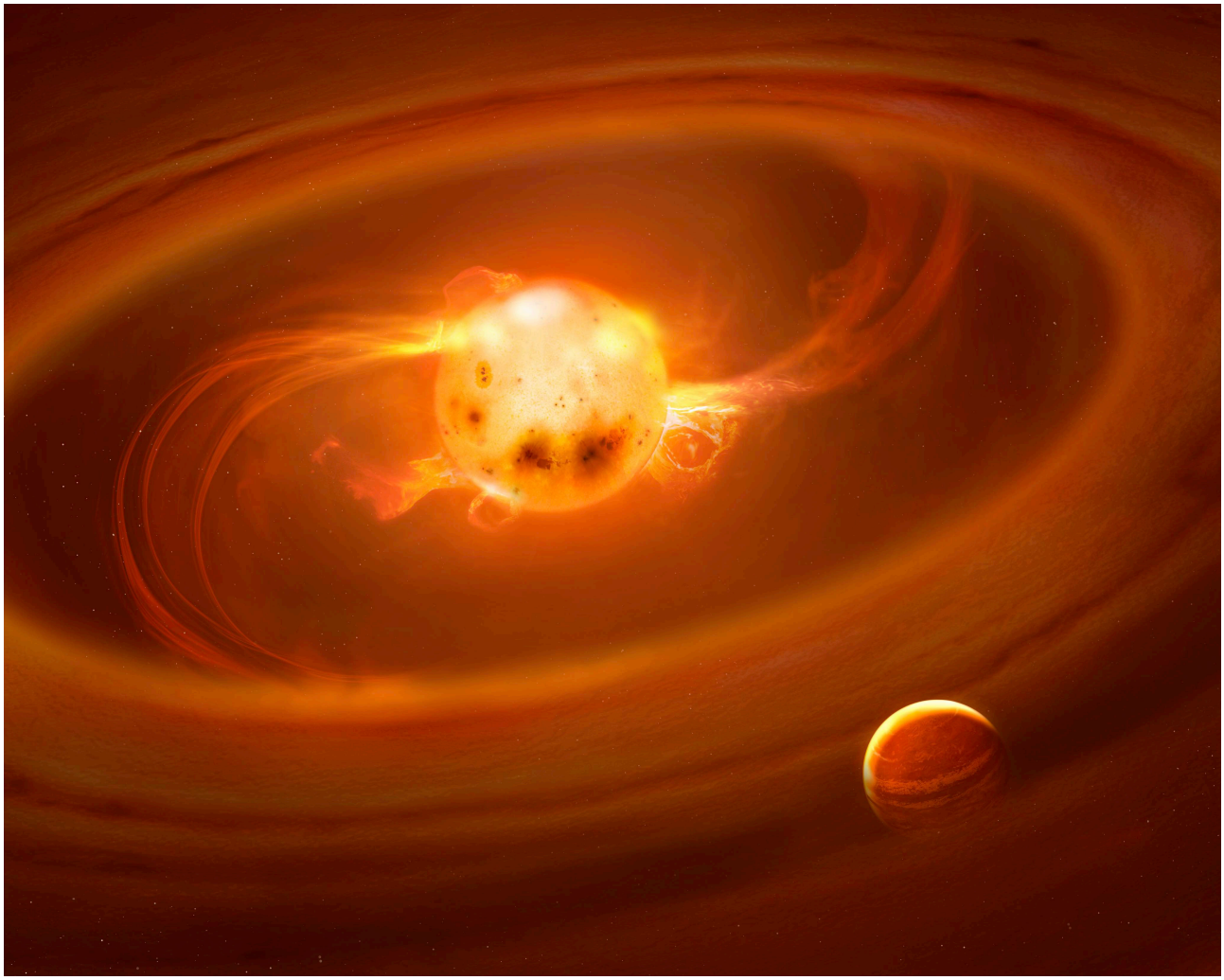
[7] https://www.qrm.de/en/products/liver-nodule- phantom/?type=3451&downloadfile=1700&cHash=86600fc915ff00055d6d267d36105e7b

Project 2. Using ESO-VLT to peer into the accretion history of young stellar objects

Assist. Prof. Rebeca Garcia Lopez

Stars form by accreting material from their surrounding protoplanetary disks. Astronomers believe that accretion takes place as matter flowing through the disk is channeled onto the stellar surface by the stellar magnetic field shocking the stellar surface at free-fall velocity. This process is called magnetospheric accretion and it represents the theoretical framework of disk accretion, that is, how stellar embryos gather mass from its surrounding disk (i.e. accrete) to become a fully grown up star.

In this project, you will study how young stars gather mass using state -of-the-art data from the European Souther Observatory (ESO). You will learn how to reduce and analysed spectroscopic data, as well as how to use gas tracers present in the spectra to peer into the accretion history of these objects



Project 3. Energy harvesting using organic piezoelectrics

Assoc. Prof. James Rice

This project centres around the design and study of an organic piezoelectric system. The project will involve the creation of the chip and the study of its power output. Deploying with pico-amp sensitivity the electrical power output from the system. This project will interest those wishing to study nanoscale materials and sustainable energy systems.

Project 4. Green photonic materials

Assoc. Prof. James Rice

This project centers on studying the optical and electrical properties of nanostructured arrays formed on lightweight and flexible thin films. Examining the optical reflection and electrical conduction processes in such systems. This project will interest those wishing to study nanophotonics and green materials.

Project 5: Extracting Biophysical Descriptors for 3D Structures: A Machine Learning Approach

Project 6: Using Nanoparticles as Drug Carriers: A Computational Study

Project 7: Quantifying non-Markovian Effects in Models of Protein Dynamics and Interactions

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Prof. Nicolae-Viorel (Vio) Buchete
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Modern computational simulations of biomolecules using high-performance computational physics (HPC), including studies of protein-protein biophysical interactions, have to overcome challenges due to the separation between the relevant physical time-scales (e.g., for protein folding or binding) and the accessible time-scales of HPC simulations. Recently, large-scale modelling methods for proteins structure and dynamics have become available due to advances in machine learning-based algorithms. Projects 1 and 2 will allow the student to explore these methods with a view (1) to extract systematically and automatically and predict physics-based descriptors of proteins,[2] and/or (2) to optimize the use of nanoparticles and nanomaterials as drug carriers for intravascular drug delivery[1].

Theoretically, we also developed new algorithms based on Coarse Master Equations (CME), where the underlying configuration space is discretized into a network of Markovian states, such that the mean lifetime of each state is much larger than the transition time between the states. Project 3 is an opportunity to learn about applying CME-based methods to the analysis of protein trajectories, such as generated using molecular dynamics (MD), and probe the limits of the Markovian assumption in designing and analysing MD simulations.[3-8]

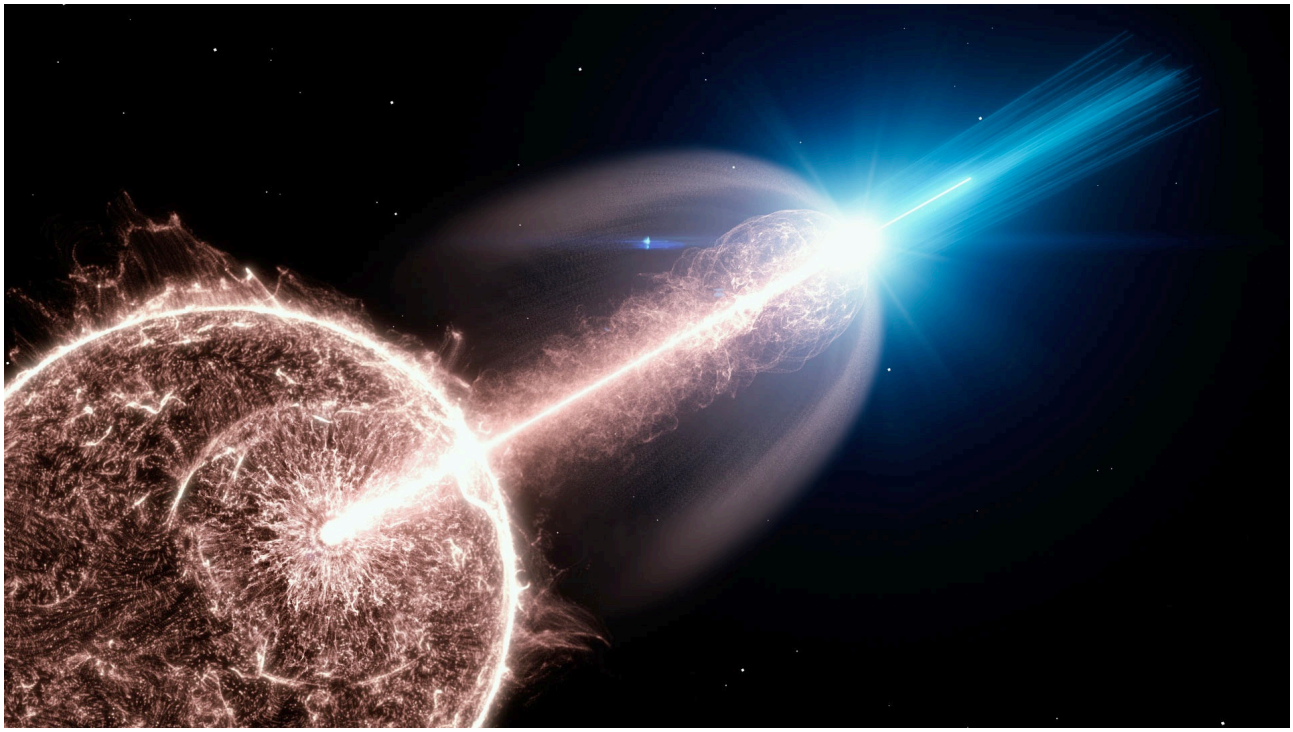
These projects (suitable to 1 or 2 students working separately, or as a team) will involve learning about computational modelling of protein structure and dynamics, about modern Markov-based stochastic statistical physics methods, running simple Matlab and/or Python codes for analysis, and/or designing and running simple molecular dynamics (MD) simulations using the CME-based formalism, using Linux workstations and supercomputing clusters, with the aim to improve the speedup of typical MD runs. Applications will study simple MD trajectories of cancer, diabetes or Alzheimer's disease-related proteins for understanding their conformational dynamics and their propensities to form oligomers and nanofibrils.[3-8]

[1] Buchete, Cicha, Dutta, and Neofytou, "Multiscale Physics-based Modelling of Nanocarrier-assisted Intravascular Drug Delivery", Frontiers in Drug Delivery, (2024) in press,(https://www.frontiersin.org/articles/10.3389/fddev.2024.1362660)
[2] Mancardi, et al., "A computational view on nanomaterial intrinsic and extrinsic features for nanosafety and sustainability", Materials Today, 67, 344 (2023) (https://doi.org/10.1016/j.mattod.2023.05.029)
[3] Narayan, Kiel, and Buchete, "Classification of GTP-dependent K-Ras4B active and inactive conformational states", J. Chem. Phys., 158 (9), 091104 (2023) (https://doi.org/10.1063/5.0139181)
[4] Narayan, Yuan, Fathizadeh, Elber, Buchete, “Long-time methods for molecular dynamics simulations: Markov State Models and Milestoning” in *Prog. in Molecular Biology and Translational Science*, Academic Press: 170, 215-237 (2020)
[5] Narayan, B; Herbert, C; Yuan, Y; Rodriguez, B; Brooks, BR; Buchete, NV (2018) 'Conformational kinetic analysis of replica exchange MD: T-dependent Markov networks for FF amyloid peptides'. *J. Chem. Phys.* 149 (7), 072323 (2018)
[6] Martini, L; Kells, A; Covino, R; Hummer, G; Buchete, NV; Rosta, E; 'Variational Identification of Markovian Transition States'. *Phys. Rev. X*. 7 (3):031060 (2017)
[7] Leahy, CT; Murphy, RD; Hummer, G; Rosta, E; Buchete, NV; *J. Phys. Chem. Lett.*, 7, 2676-2682, (2016)
[8] Buchete, NV; Hummer. G; *Physical Review E (Statistical, Nonlinear, and Soft Matter Physics),* 77, 030902 (2008)

Project 8: The fast and furious: the environments of the most violent explosions in the Universe

Assist. Prof. Antonio Martin-Carrillo

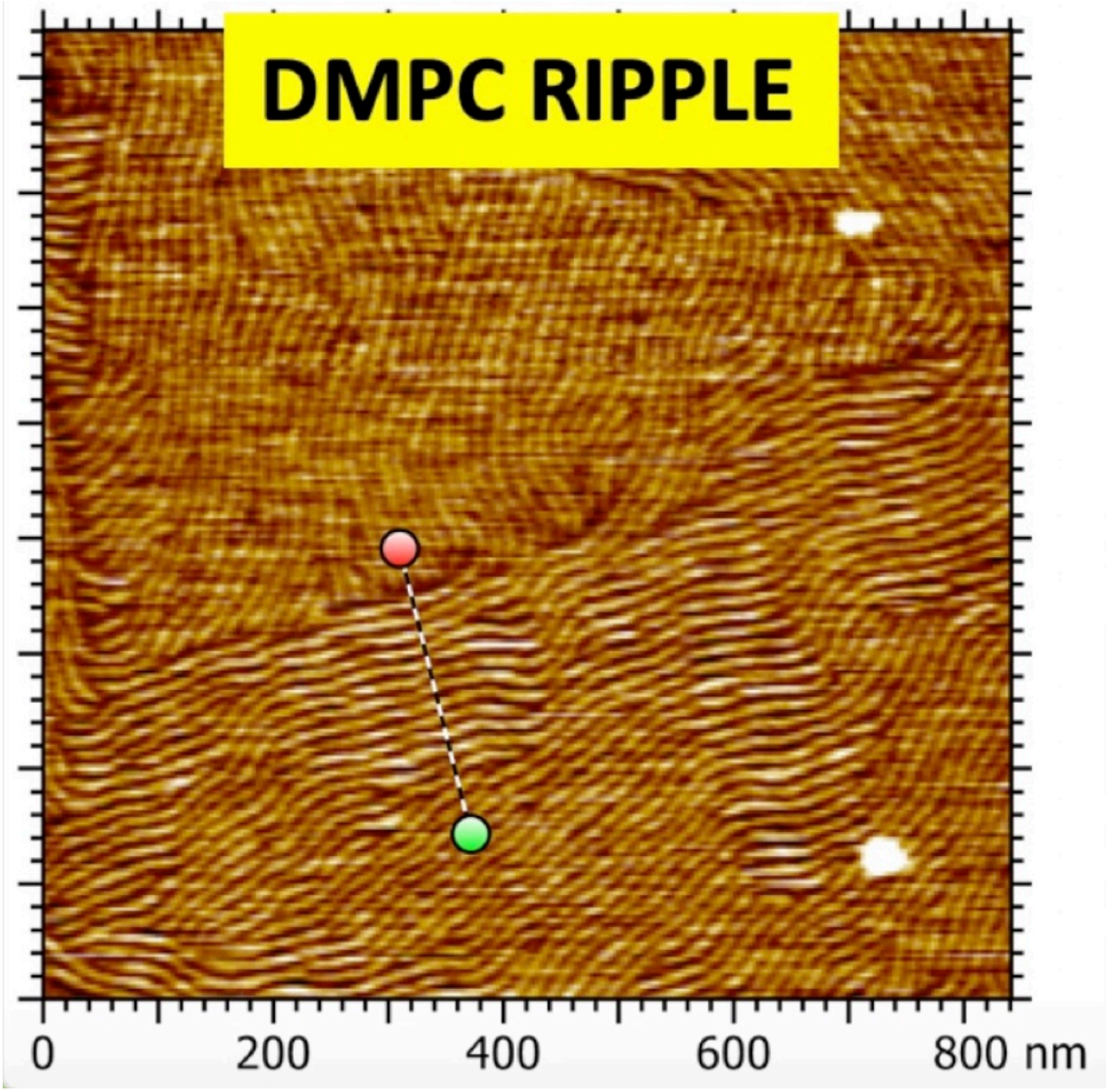
The aim of this project is to study the environments of gamma-ray bursts (GRBs) associated to supernovae by modelling GRB afterglow emission and X-ray spectra. GRBs are the most luminous explosions in the Universe, with central engines which drive the outbursts in highly relativistic jets. While the prompt emission in gamma-rays last a few seconds, the multi-wavelength afterglow can be detected even months after the main event. GRBs are known to be associated to stripped envelope massive stars via their association with a sub type of Ic supernovae. This association has led to think that the progenitors of GRBs are stars known as Wolf-Rayets. These stars suffer considerable mass loss over the last part of their lifetime. The ejected mass enriches the environment around the star and it is expected that the density of this circumburst environment is stratified, not homogeneous. However, observable evidence from GRB data seems to suggest that the environment around GRBs is indeed homogeneous. The student will be using data from space observatories such as Swift and ground-based telescopes to model the afterglow and X-ray spectra of GRBs with known supernova associations to study this discrepancy. The student will acquire valuable knowledge on the areas such as scientific computation using Python, numerical simulations, high-energy observational and theoretical astrophysics and high-energy observational techniques.



Project 9: Controlling the elasticity and viscosity of biomembranes and live cells by complex salts - An atomic force microscopy experimental study

Assist. Prof. Antonio Benedetto

The elasticity and viscosity of the cellular membrane are playing a key role in a number of processes relevant for life and in diseases. For example, it is well-known that cancer cells are softer than their healthy counterparts, which allows them to spread. Moreover, making healthy cells softer can help in wound closing. As a result, controlling the elasticity and viscosity of live cells can lead to breakthrough applications in medicine and pharmacology. In our NanoBioPhysics Lab, we are studying how the family of complex organic salts known as "ionic liquids" can be used to control bio membranes' viscoelasticity - our main technique is atomic force spectroscopy, which we combine with neutron and light scattering approaches, and a number of cell biology assays. During the internship the intern will be trained in basic and advanced atomic force spectroscopy modes for both imaging and mechanical characterisation of model biomembranes (lipid bilayers) and live cells. The effects of two ionic liquids on a model biomembrane and a model cell line will be investigated. If time allows, fluidFM technology will be also used. For more info on our Lab visit www.antoniobenedetto.eu



Project 10: Preparation of aligned collagen films and peptide nanotubes for topographical, electromechanical, electrostatic, and pyroelectric characterisation

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Prof. Brian Rodriguez

Piezoelectricity, a fundamental phenomenon wherein an electric charge is generated in response to mechanical stress, holds transformative potential for applications ranging from biomedical engineering to wearable technology. Our summer internship project is dedicated to exploring this potential in natural and bioinspired piezoelectric materials through the preparation of aligned collagen films and peptide nanotubes, respectively, and subjecting them to comprehensive analyses including topographical, electromechanical, electrostatic, and pyroelectric characterization. The intern will gain hands-on experience with the operation of Atomic Force Microscopy (AFM), delving into the most advanced piezoresponse and electrostatic response measurements at the nanoscale. As part of the Nanoscale Function Group at University College Dublin, the intern will join a multidisciplinary team pioneering innovations at the intersection of biology and nanotechnology. For more information about our group and the impactful work we do, please visit our website at https://www.nanofunction.org/. This program represents a unique opportunity to contribute to cutting-edge research while developing invaluable skills in nanotechnology and materials science. Example Kelvin probe force microscopy contact potential difference images of biased peptide nanotubes (PNTs) without (top) and with graphene oxide ‘doping’ (bottom) are shown below.