First HPC@QMUL Annual User Meeting

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Agenda

9:00 a.m. Registration

9:30 a.m. **IT Manager:** Welcoming words

9:45 a.m. **Qilei Li:** Person ReID

Person re-identification (ReID) is a computer vison task that aims to identify individuals across various locations and time frames using images or videos collected from widely distributed camera networks. This task is fundamental in surveillance and security applications, where consistent tracking of individuals across different environments is crucial. Accelerated by deep learning, ReID extracts reliable features that enable accurate person searches within large-scale datasets. However, these models face the challenge of generalizing effectively across data from diverse domains, each with unique visual characteristics and distribution patterns.

Ensuring generalizability requires advanced representation learning strategies that can bridge these domain gaps, allowing ReID models to perform robustly in new environments. High-performance computing (HPC) becomes essential here, as it provides the computational power needed to train and fine-tune these models on massive datasets.

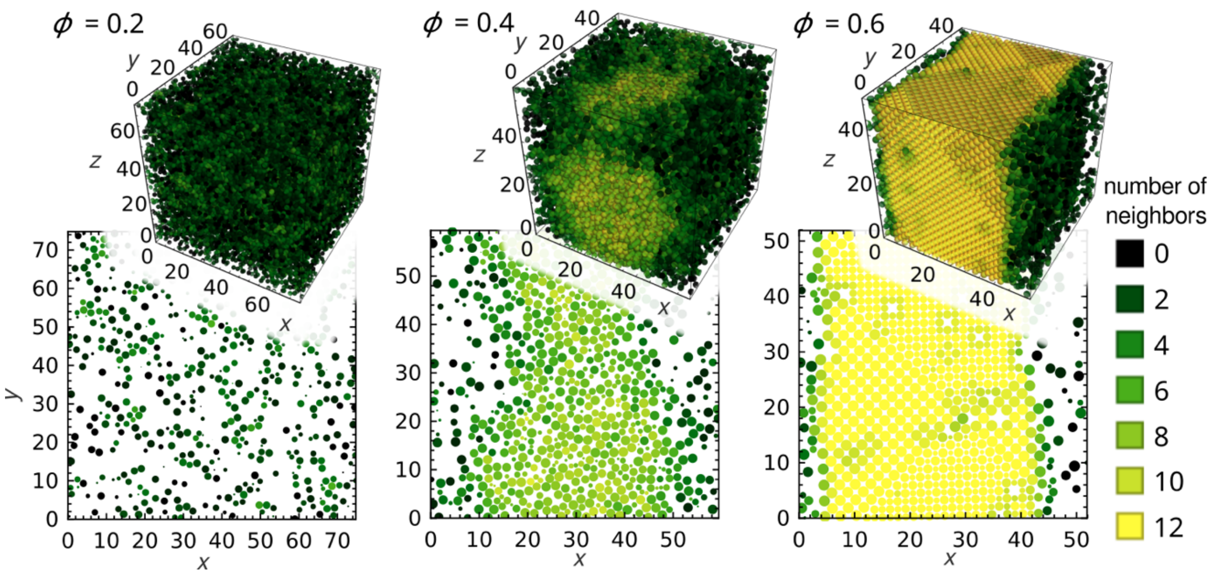
This capability enhances the scalability and adaptability of ReID, allowing models to process and analyze data from vast, dynamic sources, ultimately ensuring more reliable and precise person identification across complex real-world scenarios.

10:15 a.m.

Lennart Dabelow

Macroscopic regularity from microscopic complexity

It is a fascinating empirical fact that macroscopic systems often exhibit surprisingly stable and regular behavior despite the vastly complicated dynamics and interactions of their microscopic constituents. My research combines analytical and numerical methods to understand this emergence of macroscopic regularity from microscopic complexity in various frameworks, from quantum systems to mesoscopic biological and artificial swimmers to machine-learning models. In this talk, I will exemplify this with a recent result about so-called active-matter systems, such as bacteria, catalytic colloids and nanorobots. I will show how the microscopic irreversibility of their observable dynamics can be related to macroscopic thermodynamic state variables.

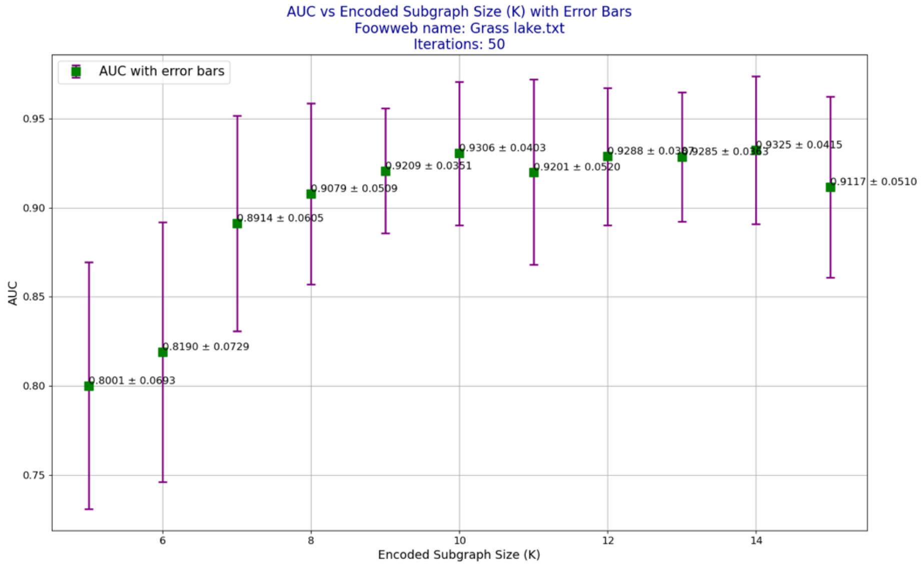


10:45 a.m. Jorge Eduardo Castro Cruces

The effects of climate change are intensifying globally, driven by severe weather events that have resulted in the decline of numerous species. It is imperative to obtain precise insights into the threats posed to our ecosystems, enabling us to effectively manage and potentially alleviate further environmental deterioration in the future. Ecological interconnectedness plays a crucial role in anticipating responses to climate change, as the decline of a single species can cascade through the network, impacting the populations of its predators or prey as species adapt to shifting environmental conditions. Fortunately for us, this project endeavors to enhance our comprehension of how Global Environmental Change (GEC) disrupts ecological networks and redefines community organization.

Leveraging machine learning techniques, we aim to unravel the structural and re-assembly principles governing ecosystems under stress. By employing advanced graph data science, we will decode topological characteristics and forecast species adaptation and rewiring in response to climate change.

Our model will pioneer a predictive framework to anticipate ecosystem-level responses, providing evidence-based guidance for conservation interventions. Furthermore, this research contributes to the burgeoning field of ecoinformatics by offering novel methodologies for deciphering vast ecological datasets. Through these endeavors, we strive to empower stakeholders with tools to navigate the complexities of ecosystem resilience in the face of environmental change.



In conclusion, this research outlines a comprehensive plan to predict new links and ecosystem re-assembly using machine learning techniques. The findings from this research will contribute significantly to the field of Ecology and Machine Learning, providing valuable insights into community organization and resilience in the face of biodiversity loss.

11:15 am to 11:30 am

Coffee Break

and

Networking

11:30 a.m.

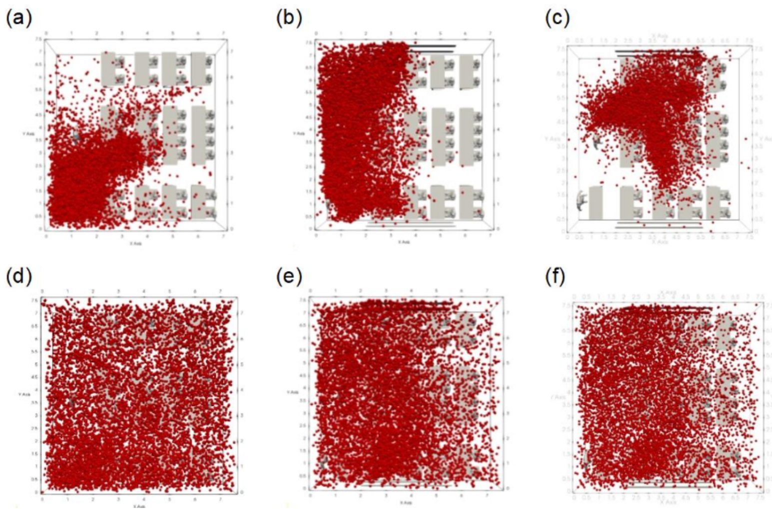
Nathan Boachie

Damage due to cavitation collapse is evident in many applications, with the most notable case being through the damage seen to propeller or turbine blades in underwater applications. For decades, the pathway under which a cavity collapsing near a surface creates a pressure high enough to damage a metal has evolved with experimental findings. The state-of-the-art research suggests an interesting result, that the damage forms under a non-axisymmetric self-focused collapse of a cavity near solid surface. My research will be attempting to reproduce this result numerically, through simulations of three-dimensional, non-axisymmetric bubble collapses near surfaces which will be novel in this field. Various multiphase flow treatments may also be applied in using a method which will yield an accurate flow resolution whilst maintaining a fair computational cost.

12:00 m. Rabia Abid

The recent Covid pandemic has highlighted the need to understand and control the air flow indoors and particularly in public settings. An important sector that has been seriously affected by the pandemic was the educational sector, where many pupils were forced to go online and have missed much of the learning experience. It is only a question of time to when humanity will have another wave of airborne diseases pandemic and thus it is of importance to prepare the tools and settings for such events. Breaking the transmission chain by reducing the pathogen load in the air through ventilation is obvious. Reduced-order modelling is commonly based on the fully mixed air assumption. Although it can lead to useful guidance such as the required level of air changes per hour (ACH), it cannot explain why there are places in the room that seem to be more vulnerable for infection and cannot provide guidance where best to place the ventilation. In this context computational fluid dynamics (CFD) that includes particle dynamics can be useful. We will present a CFD implementation in OpenFOAM using the Eulerian-Lagrangian approach. The air flow is modelled using the URANS method where people's thermal plumes are simulated using the Boussinesq approximation. The motion droplets are simulated through a Lagrangian simulation accounting for drag, buoyancy and gravity. The focus was on far field spreading and thus looking at droplet sizes of 2 and 15 microns which do not pass an evaporation phase (although such phase can be added using existing OpenFOAM tools for large droplets in the near field). A generic medium size class of two standing instructors and thirty sitting pupils is investigated, where one infector is assumed (an instructor or a pupil). A short speech of 5 seconds is simulated to study the motion of 10000 droplets, focusing on far field spreading. Two scenarios are simulated, a poorly ventilated classroom and a well venerated classroom (6 ACH).

Stark difference is observed between the two. The poorly ventilated classroom shows the dominance of the people's thermal plumes over the air flow and hence determining the droplets convection. This leaves places in the classroom which are more prone to accumulation of the droplets (and hence a higher infection risk) than others, e.g. certain corners in the room. On the other hand, the ventilation causes more uniform spreading of the droplets in early times and better protects those sitting far from the infector at later times.

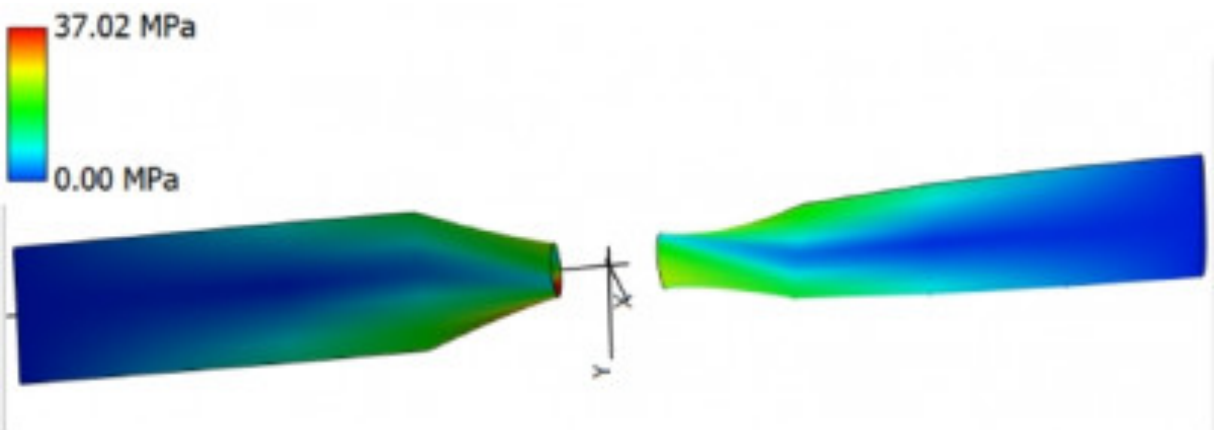


The effects of the infector's position and the level of occupation in the classroom will be discussed in the presentation as well as an infection risk analysis adapted to CFD calculations and incomplete air mixing situations.

12:30 p.m.

Omar Abdi

Small wind turbines play a vital role in the distributed terrestrial energy market and airborne applications. Unlike larger turbines, small turbines are influenced by laminar boundary layer aerodynamics, which can lead to reduced lift, earlier stall, and lower power coefficients. Enhancing their aerodynamic performance is therefore essential. This study investigates the effects of Gurney flap - small tabs attached along all or part of a blade's trailing edge on a horizontal axis wind turbine. Computational fluid dynamics (CFD) and blade element momentum (BEM) calculations show an increase in the power coefficient at higher tip speed ratios compared to a clean two-blade turbine. Structural analysis is conducted using a finite-element solver, and a semi-empirical formula is used to estimate turbine noise. The results indicate a moderate trade-off between the improved power performance achieved by the Gurney flaps installation and increased structural stress and noise, highlighting the potential benefits of Gurney flap design. This novel approach will be further investigated using the HPC resources and integrated into a system providing power for water pumping and energy storage used by small urban and rural end users.



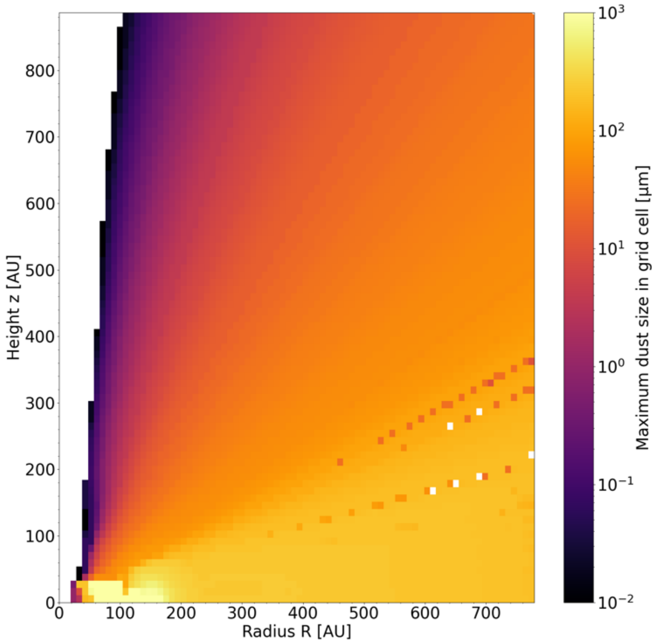
1:00 p.m. 2:15 p.m.

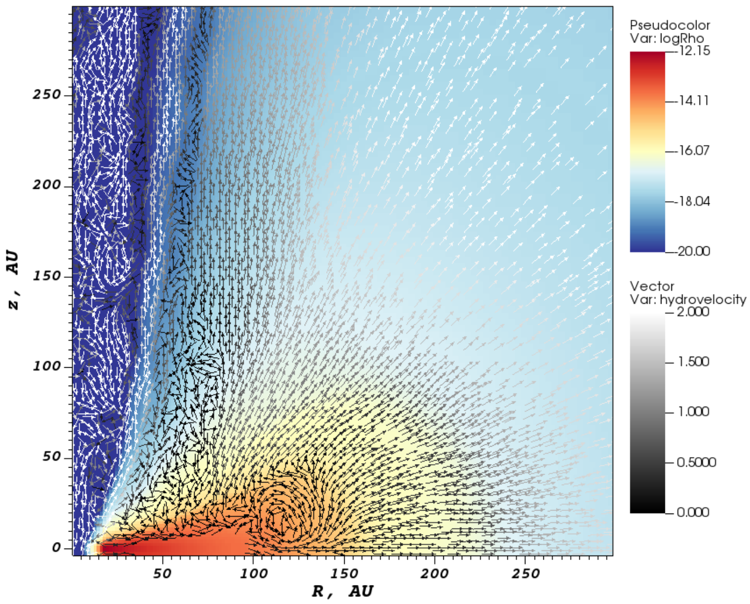
Lunch time

2:15 p.m.

Sebastien Paine

The environment in which circumstellar discs evolve plays a crucial role in their evolution, and the formation of planets. In stellar clusters, nearby large stars will irradiate gas and dust: heating the disc and entraining planet-forming materials. An important, but under-studied aspect of this is what sizes of dust get carried in the disc wind. This affects the amount and position of planet-forming solids, as well as dust shielding the disc from UV radiation. We have developed a particle solver to track the motion of dust in multi-dimensional simulations of photo-evaporating discs.

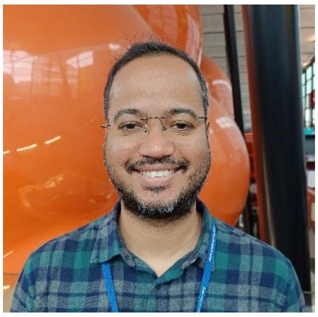




The code independently evolves 1000s of dust grains in parallel, using a golden-section search algorithm to find the maximum dust size entrained across the disc. We validate an existing analytic estimate in 1D by Facchini et al. (2016) but find the situation more complex for 2D axisymmetric models. There, dust entrainment varies significantly depending on where from the disc surface the dust is launched into the wind. However, we also find that the dust opacity is mostly uniform from all directions. This has implications for the structure of gas mass loss and observational characteristics of externally irradiated discs.

2:45 p.m.

Raju Kumar



Metabolic dysfunction-associated steatotic liver disease (MASLD) is the most common cause of chronic liver disease worldwide and accounts for over 2 million deaths per year. It is characterized by the accumulation of fat in the liver and its progressive form with inflammation and liver fibrosis. Fibrosis predicts disease outcomes, and little is known about the fibrosis factors, particularly immune cells. Patients with MASLD have metabolic dysfunction which is often associated with inflammation in the adipose tissue and the effect of this on fibrosis development is also unknown. I am characterising T cell-mediated responses in early-stage MASLD patients. We did single cell sequencing of immune cells isolated from a cohort of patients undergoing bariatric surgery for weight loss but exhibiting MASLD.

We performed CITE-Seq and TCR-Seq on immune ($CD45^+$) cells isolated from simultaneously sampled liver, blood, subcutaneous (SAT), and visceral adipose tissue (VAT) sampled during bariatric surgery in 14 patients. We used Seurat V5.1.0 and scRepertoire 2.0.4 for CITE-Seq and TCR-Seq analysis respectively.

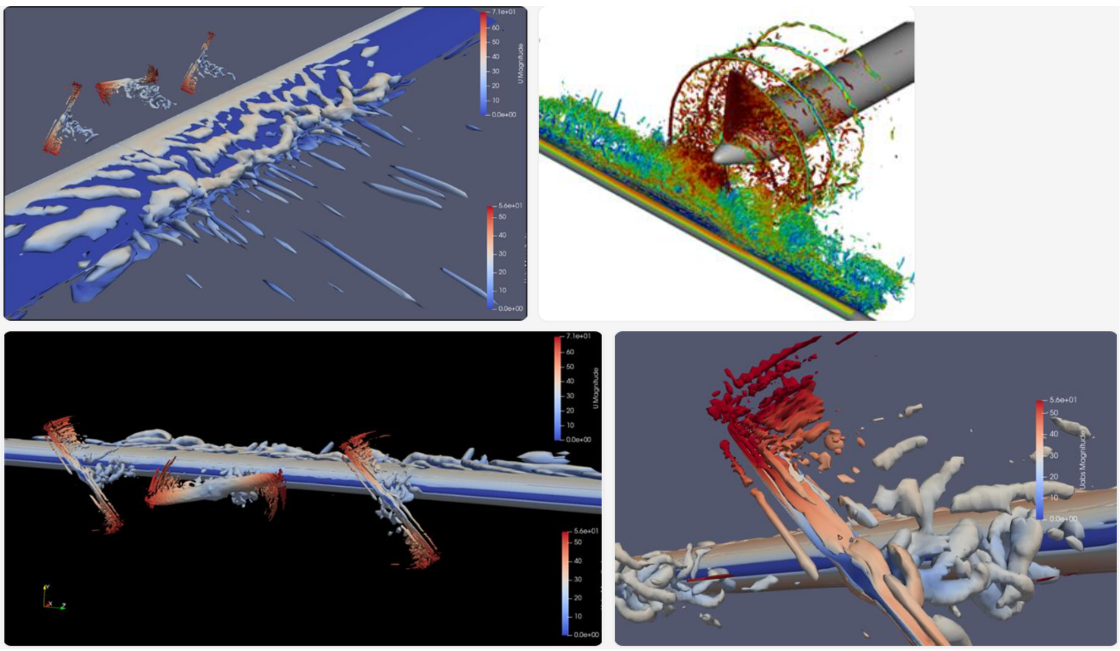
We are studying early-stage MASLD and identifying fibrosis-associated T-cell function, clonality, and candidate immune epitopes. F1-2 patients' T cell clones are inflammatory, selected, expanded, and can be identified in different tissue compartments.

3:15 p.m.

Hussain Ali Abid

The talk will highlight advanced computational methods for modelling and mitigating noise in modern propulsion systems, with a focus on applications in Urban Air Mobility (UAM). Particular emphasis will be placed on the CABARET scheme for rotating grids, which leverages GPU-accelerated asynchronous time-stepping to enable efficient simulations of complex aerodynamic and acoustic phenomena. The discussion will also explore the integration of sliding mesh interfaces, demonstrating their critical role in enhancing computational efficiency and accuracy by redefining conservation fluxes across moving and stationary zones.

The presentation will explore boundary layer ingestion concepts aimed at improving propulsion efficiency, supported by experiments involving a two-bladed propeller immersed in a thick boundary layer. Computational results, validated against experimental findings, illustrate how refined grids (up to 5 million cells) can effectively predict tonal and broadband noise at frequencies up to 5 kHz. Additionally, the talk will address distributed electric propulsion systems by presenting sensitivity studies on noise reduction strategies. These include the influence of serrated trailing edges, rotor phase shifts, and propeller positioning. The findings reveal that optimal configurations can achieve noise reductions of up to 5 dB, aligning with UAM's regulatory, environmental, and market objectives. This research highlights the potential of high-resolution, GPU-driven tools for developing quieter, more sustainable propulsion systems tailored for future smart cities.



3:45 pm to 4:00 pm

Coffee Break

and

Networking

4:00 p.m.

Siqhi Lu

Depression in adolescents is a growing public health concern worldwide, posing a significant cost to families and society. Recent emphasis has been placed on the prevention of depression in adolescence, rather than treatment. However, studies have focused on relatively small samples and a limited number of predictors. Depression is a complex, multidimensional condition that necessitates comprehensive investigations into its risk factors. These studies must consider a wide range of potential contributors and often require computationally intensive modelling working with high-performance computing (HPC) environments.

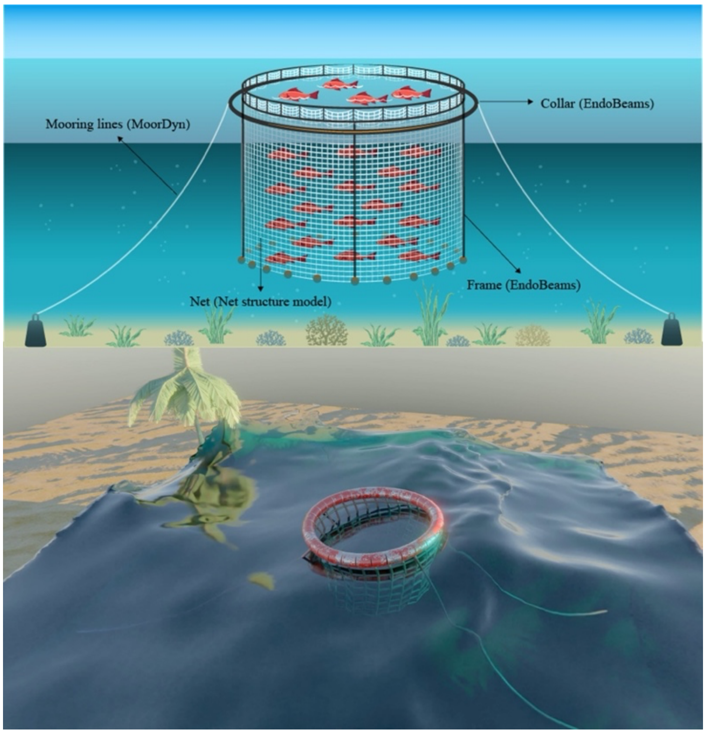
My research aimed to examine the predictors of adolescent depression in a large, sociodemographically diverse sample with nearly 5000 children aged 9-10 years old. They completed follow-up assessments after 3 years. To predict depression at follow-up, we employed machine learning algorithms including support vector machine (SVM), random forest and elastic net. This prediction model incorporated a wide range of risk factors measured at the baseline assessment, including cognition, mental and physical health, and environment. It will provide a deeper understanding of the mechanisms leading to adolescent depression, with implications for early identification and prevention of these outcomes in those at the highest risk.

4:30 p.m.

Mi Shuo

A new integrated numerical framework is developed for simulating he fluid-structure interaction of aquaculture systems. The framework is based on our previous OpenFOAM formulation [1], while being coupled with a lumped mass-mooring model, MoorDyn [2], and a finite-element structural solver, EndoBeams [3]. The turbulent flow is taken as incompressible fluid solver and solved using a volume of fluid surface capturing method. The motion and deformation of the flexible nets are calculated using the screen and mass-spring methods.

MoorDyn is used for simulating mooring lines while EndoBeams are used to calculate the deformation of other components of the aquaculture system, such as collars and frames. The coupling of all the components follows a loose-coupling method.



The immersed boundary method is employed for the interactions between the fluid and all components of the aquaculture system.

Fluid particle dynamics is also modelled using the Eulerian-Lagrangian to simulate fish disease waterborne transmission within aquaculture system area. The framework has been validated with extensive experimental data from the literature and is demonstrated as a robust tool to simulate the complex fluid-structure-particle dynamics of aquaculture systems.