

OLLSCOIL NA GAILLIMHE UNIVERSITY OF GALWAY

Coláiste na hEolaíochta & na hInnealtoireachta College of Science & Engineering

RESEARCH AND INNOVATION DAY 2024

CURIOSITY & DISCOVERY

DECISIVE DATA

INNOVATION FOR HEALTH

SUSTAINABLE FUTURES





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CURIOSITY & DISCOVERY

DECISIVE DATA

Oral Presentations



Abstract

Patterns UI, an Interactive Tool for Music Exploration Sweeney, R.1, Jajoria, P.1, Diamond, D.1, D'Aquin, M.2, McDermott, D.1. 1. Data Science Institute and School of Computer Science, University of Galway, Ireland 2. Jab matrixed particular de Dachard have a la formation and the direction and the direct

2. Laboratoire Lorrain de Recherche en Informatique et Applications and Institut des Sciences du Digital, Université de Lorraine, Nancy, France

INTRODUCTION

Patterns UI is a user interface intended as a tool for musicologists, musicians and lay users to explore traditional music corpora through visualisations of tunes and shared melodic patterns. Melodic patterns are short, integer n-grams representing a sequence of accented notes. The application was developed as a part of the Polifonia EU Horizon 2020 project. It is available online at https://polifonia.disi.unibo.it/patterns.





MATERIALS AND METHODS

A co-design process involving a competitor analysis of similar interfaces, and remote, semistructured interviews with musicologists was used to establish requirements.

Patterns UI is composed of a frontend written using the Vue.js JavaScript framework and a backend written using the Python Flask web framework. The backend queries an RDF knowledge graph as a source of pattern data and tune metadata.

A central feature is an interactive network visualisation showing tunes, patterns, and the relationships among them, as shown in Fig 1. The interface also features a fuzzy search for tunes by title, a search by pattern, and an 'Advanced' search comprising the aforementioned search fields in addition to dropdown fields for 'Corpus', 'Key', 'Time Signature' and 'Tune Type'.

A search results link to a 'Composition' page featuring the interactive network visualisation and interactive tabular pattern data for the selected tune. 'Tune Family' pages list related tunes and 'Pattern' pages present a selected pattern on a stave and as audio.

RESULTS AND DISCUSSION

The Patterns UI interface was evaluated through in-person and remote usability testing with domain-expert users and a remote walkthrough demonstration with Polifonia consortium members. The evaluations resulted in positive responses and some useful feedback.



Abstract

3D Imaging of Micro-particles Launched from Custom MEMS Devices Using a GRIN-lensbased In-line Digital Holographic Microscope

Khorshad, A. A.¹, Devaney, N.¹

¹Applied Optics group, Physics unit, School of Natural Sciences.

INTRODUCTION: Our research project entitled "MEMS-based Nano-particle storage and release system for Quantum Physics payload Platform (QPPF)" (MEMS4QPPF) is a collaboration with Tyndall National Institute (TNI) and fully funded by the European Space Agency. The final aim of the MEMS4QPPF project is to demonstrate a Micro-Electro-Mechanical System (MEMS) storage and release device capable of loading massive 100nm diameter silica particles into an optical trap where they can be cooled and released for matter-wave interferometry aimed at testing the transition from quantum physics to classical physics in space (a perfect vacuum and perturbation-free medium). To this end, different types of MEMS devices have been developed by the TNI and then tested with a GRIN-lens-based in-line Digital Holographic Microscopy (DHM) system, which we have developed, both theoretically and experimentally, here at University of Galway over the past two years. Experimental results show that the smallest spherical silica particles that can be released from the current MEMS devices are about $4\mu m$ in diameter.

MATERIALS AND METHODS: A variety of different 3 by 3 arrays of flexural silicon membranes, monolithically integrated with $1\mu m$ thick aluminium nitride piezoelectric layers, were fabricated as the MEMS devices by the TNI using silicon-on-insulator micromachining technology and then wire-bonded to Printed Circuit Boards (PCBs). Fig. 1(a) shows a typical PCB, where the side length and thickness of the 9 visible square membranes are $400\mu m$ and $8\mu m$, respectively. If the membranes are actuated (through the pins on the board) with a sine wave of proper amplitude and at their exact resonance frequencies, then micro-particles, pre-loaded onto the membranes with a micropipette, are launched. Fig. 1(b) presents an inline configuration of DHM technique we have developed to automatically detect, track and measure the size and velocity of launched micro-particles. In this setup a radial-GRIN rod lens has been utilized that provides advantages compared to the conventional pinhole-based DHM systems. All optical components and the PCB are setup inside a vacuum chamber in order to significantly reduce the air resistance experienced by released micro-particles. A high-speed camera is vertically positioned over the chamber output window in order to record the holograms required for further image reconstructions.

RESULTS AND DISCUSSION: Various PCBs of the MEMS devices, loaded with different particle sizes (from 900*nm* to 300 μ *m*), have been tested with the setup shown in Fig. 1(b). Fig. 1(c) demonstrates a 2D projection image of monodisperse 10μ *m* particles launched by a typical MEMS device. The smallest particle released and imaged using the above-described technologies is about 4μ *m* and it is expected to be even smaller if the surface of the membranes are modified.



Figure 1: (a) An array of MEMS devices attached to a PCB, (b) The combination of DHM system and a vacuum chamber, (c) A sample image of the released $10\mu m$ particles.



Abstract

Genome-wide CRISPR/Cas9 Loss-of-Function Screens Reveal Genes that Determine Cell Responses to CDC7 Kinase Inhibitors
Centre for Chromosome Biology, School of Biological and Chemical Sciences,
University of Galway
INTRODUCTION

CDC7 kinase is a key regulator of initiation of DNA replication. Several CDC7 inhibitors (CDC7is) have been developed as anti-cancer drugs, however, their anti-proliferative activity greatly varies across cell-types indicating that genetic background influences how cells respond to the drugs.

METHODOLOGY

We aim to identify the genes that determine the cell responses to CDC7is using a CRISPR/Cas9 genome-wide loss-of-function screening platform we have established. Our workflow utilizes a breast-derived cell line expressing Cas9 (MCF10A^{EditR}) and a pooled lentiviral-vector library consisting of 155,000 sgRNAs targeting ~19,000 protein encoding genes.



RESULTS AND DISCUSSION

In a pilot screen, MCF10A^{EditR} cells were infected with the library and then treated with a high dose of CDC7i that strongly inhibits cell proliferation. sgRNA representation before and after treatment was determined by next-generation sequencing, revealing genes that upon editing, allow cells to grow better in presence of the CDC7i. Among these hits was ETAA1 an activating subunit of the replication stress-response kinase ATR. We show that ETAA1 with ATR is important to restrain replication origin activation and to prevent mitotic catastrophe when CDC7 function is impeded¹.

A much large screen now identifies ~270 genes that upon editing either enhance resistance or sensitize cells to CDC7is. CDK8, a kinase previously associated only with transcriptional regulation, is the top sensitizer. We find that the synergistic effect of CDC7 and CDK8 inhibition on cell proliferation is related to the decrease in the rate of DNA synthesis, linking CDK8 also to regulation of DNA replication. Ongoing studies are uncovering the molecular mechanism by which CDK8 together with CDC7 regulates DNA replication.

Our results increase understanding of how human DNA replication is regulated and point to targets and possible drug combinations that may enhance the activity of CDC7i.

¹Rainey, M.D. *et.al:* ATR Restrains DNA Synthesis and Mitotic Catastrophe in Response to CDC7

Inhibition.Cell.Rep.32.(2020).DOI:10.1016/j.celrep.2020.108096.



Abstract

STRAND-SPECIFIC OXIDATIVE DAMAGE ARTEFACTS IN TCGA WHOLE-EXOME SEQUENCING SAMPLES	
Medina, T ^{1,2} , Bennett, D ¹ , Seoighe, C ¹ .	
1. School of Mathematical and Statistical Sciences, University of Galway, Galway,	
2. SFI Centre for Research Training in Genomics Data Science, Science Foundation	
Ireland, Dublin, Ireland	
	STRAND-SPECIFIC OXIDATIVE DAMAGE ARTEFACTS IN TCGA WHOLE-EXOME SEQUENCING SAMPLES Medina, T ^{1,2} , Bennett, D ¹ , Seoighe, C ¹ . 1. School of Mathematical and Statistical Sciences, University of Galway, Galway, 2. SFI Centre for Research Training in Genomics Data Science, Science Foundation Ireland, Dublin, Ireland

INTRODUCTION

Oxidative damage to DNA can cause G>T mutations via an 8-oxo-guanine (8-oxo-G) intermediary. These mutations often arise as technical artefacts during DNA sequencing but are distinguishable from biological mutations by their asymmetric occurrence by DNA strand. These artefacts can produce false positive variant calls, but current methods exist to filter 8-oxo-G artefacts, such as the FoxoG metric. While this phenomenon has been recognized and addressed, biases influencing the direction of asymmetry have not.

MATERIALS AND METHODS

We investigated strand-specific mutation bias in whole-exome sequencing data from 706 tumour samples from 9 cohorts of The Cancer Genome Atlas (TCGA), each sequenced with the same capture kit. We first calculated the ratio of reference strand versus non-reference strand alignment mismatches, per single base substitution (SBS) type, per sample. We then calculated similar ratios for each sample's variant calls to identify any evidence of similar biases in somatic genotyping, and checked for correlation between the two metrics.





RESULTS AND CONCLUSIONS

Of the 6 SBS types, G>T mismatches exhibited the greatest strand-specific bias by far, occurring more than twice as often on the reference strand (Fig. 1). Similarly, G>T variant calls occurred twice as often as their complements on average. Though this call imbalance is greatly reduced by FoxoG filtering, we found a significant correlation between G>T mismatch and passing variant ratios, suggesting the presence of residual artefacts in tumour genotypes, and found that in the testicular germ cell tumour cohort, twice as many passing G>T variants are found compared to C>A. This work highlights the need to account for strand-specific biases introduced by capture kits, particularly for applications reliant on low-frequency mutations such as tumour sequencing.



Abstract

Efficient Key-Frame Sampling Using Frobenius Norm for Video based Activity Recognition

Tchangmena1 A Nken Allassan, Mckeever2 Susan., Corcoran1 Peter, Ullah1 Ihsan

- 1. School of Computer Science, University of Galway, Galway, Ireland
- 2. School of Computer Science, Technological University of Dublin, Dublin, Ireland

ABSTRACT

This paper introduces what we believe to be the first key-frame sampling technique that utilizes the statistical distribution of classes, to identify key frames within a HAR dataset. Our approach leverages the Frobenius norm to detect salient changes across video frames. Specifically, by computing the mean Frobenius norm within each class of activity, a periodic trend is unveiled that encapsulates valuable information about the natural sampling rate of frames inherent to each activity class. Our experimental results demonstrate the efficacy of our sampling technique, showing 2% improvement of top@1 accuracy on average over uniform sampling and fixed stride sampling in fine-tuning tasks across 3 activity recognition datasets. Our experimental results are comparable in accuracy to existing state-of-the-art, whilst reducing frames and processing time by 70 - 93.75% compared to all frames video based HAR .

INTRODUCTION

Efficiently identifying key frames in video-based Human Activity Recognition (HAR) is a significant challenge, as these frames represent global information capturing scene changes and different activities, crucial for achieving high classification performance and deriving efficient video representations, with previous research exploring various methods from detecting salient changes to employing deep learning techniques like attention mechanisms. In this study, we aim to develop a scalable and computationally efficient solution for human activity recognition by leveraging statistical distribution to intelligently sample key frames, particularly targeting resource-constrained environments like edge devices, while maintaining high recognition accuracy.

MATERIALS AND METHODS

The motion difference between consecutive frames in a video clip is quantified using the Frobenius norm, visualized as a bar plot where each bin represents the level of variation between adjacent frames, with higher peak values indicating potential key frames signifying significant changes within the video sequence. When performing an average of the degree of variations across all the videos of the specified class, we obtain a smooth variation with periodic peaks across the frame sequence. These peaks are a strong proxy for key-frames identification.



Figure 1 : Average Frobenius norm

RESULTS AND DISCUSSION

By comparing our approach with two commonly used frame sampling techniques—uniform frame sampling and fixed-stride sampling—we observed a performance improvement of video top@1 accuracy of 2% across three video activity recognition datasets (UCF-101, HMDB51, and Toyota-Smart Home dataset). Additionally, we benchmarked our sampling strategy against other state-of-the-art (SOTA) techniques, including those implemented in the temporal segmentation network (TSN), SMART, and motion-guided sampling (MG-Sampler). Our results indicate that our approach delivers comparable performance to these SOTA samplings.



Abstract

A comprehensive review of algorithms and evaluation metrics for the generation of synthetic	
transcriptomic data	
<u>Haseja, D</u> ¹ , Ó Broin, P ¹ .	
1. School of Mathematical & Statistical Sciences, University of Galway, Ireland.	

ABSTRACT

In recent years, there has been increased interest in the generation of synthetic data for use in biomedical research and precision medicine. This interest has partially been driven by the EU GDPR directive for health data anonymization and pseudonymization, based on the draft European Health Data Space (EHDS) Regulation[1], which focuses on securing sensitive personal information, in particular confidential healthcare data[2].

Generating synthetic data which can sufficiently recapitulate the underlying characteristics of the real datasets from which they are created can allow researchers to overcome some of the limitations of sharing restrictions on real data, such as providing sufficient power for statistical models or ensuring adequate training dataset sizes for machine learning algorithms.

In the field of transcriptomic research, simulation of artificial bulk RNA-Seq and scRNA-seq data can be used especially for the purpose of genetic expression analysis, isoform expression analysis and enrichment analysis[3]. This can have wide ranging applications in the field of biomarker identification, novel therapeutic discovery and functional pathway research[4].

The main objective of this study is to review the underlying statistical models and/or generative algorithms used to create some of these datasets, and to survey the evaluation metrics commonly used to benchmark their similarity to the underlying real data.

This project is part of an initiative by the ELIXIR machine learning focus group[5] to assess the usage and utility of a wide range of synthetic data types across the biomedical research community.

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AŁ	ostr	act

ARFQA-HCKAN: Multi-domain Question Answering System with Heterogeneous CKANs and
Large Language Models

Al-Qatf, M¹, Alsamhi, S¹, Haque, R¹, and Curry, E¹

1. Insight Centre for Data Analytics, University of Galway

INTRODUCTION

Large language models (LLMs) have demonstrated extraordinary capabilities on diverse tasks, primarily question answering (QA). However, LLMs face several challenges, such as hallucinations, lack of novelty in knowledge, outdated knowledge, and privacy and security concerns. Some previous retrieval-based frameworks have been proposed as a promising solution to improve LLMs by integrating external knowledge bases. However, the external knowledge bases are limited and collected randomly from several new datasets that can be biased to specific domains. To address this issue, we propose a novel Adaptive retrieval-augmented framework-based multi-domain question answering System with heterogeneous comprehensive knowledge archive networks (ARFQA-HCKANs) and LLMs.

METHOD

In the proposed framework, CKAN, which is an open-source data management system designed to facilitate the storage, sharing, and management of large datasets, plays a vital role in achieving high security and privacy while retrieving and supporting accurate answers of the LLM-based QA system. We merge the dynamic knowledge of the heterogeneous CKANs and the intrinsic knowledge of LLMs to obtain the accurate final answer to the given question. Adaptive retrieval-augmented approach can guide the LLMs in deciding the necessity of external knowledge retrieval. A heterogeneous CKAN-based retrieval method is proposed to fetch external knowledge from multiple CKAN instances. To ensure the relevance of retrieved knowledge with the given question, the proposed framework introduces a reweighting method between the retrieved external knowledge and LLMs knowledge. The Figure below illustrates clearly our proposed framework.



Figure 1: ARFQA-HCKAN Framework

RESULTS AND DISCUSSION

This is an ongoing research that will result in ARFQA-HCKAN framework that represents a novel method to enhance the LLMs for QA through integrating dynamic knowledge from heterogeneous CKANs with the intrinsic knowledge of LLMs as well as considering privacy and security concerns during the external knowledge retrieval process.



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College of Science and Engineering, Research and Innovation Day 2024 - Abstract

A Cross-Sectional Analysis of Design Principles Across Critical CSA Documents in Data Spaces

Razzaq, Muhammad Asif₁; Haque, Rafiqul₁; Curry, Edward₁

1. Data Science Institute, Insight Centre for Data Analytics

ABSTRACT

This comprehensive study delves into the details of missing design principles across eight critical Collaborative Research Actions (CSA) documents, each pertaining to distinct domains within the Data Spaces. Through a careful cross-sectional Gap Analysis, this study dissects every design principle, spotlighting the specific aspects where crucial details are absent. By identifying these gaps, the study also serves as a roadmap for enhancing the robustness and completeness of the design principles, ensuring a more comprehensive framework for addressing diverse challenges in the multifaceted landscape of the Data Space.

INTRODUCTION

Various CSA initiatives focus on integrating business, use case, and data product development, emphasizing strategic practices, but require further refinement to address specific aspects such as data space intermediaries, regulatory compliance, and data interoperability comprehensively.

MATERIALS AND METHODS

The three-stage validation process outlined in Fig. 1 emphasizes robustness and stakeholder alignment in datadriven initiatives. Validation I, **Requirement Validation, ensures** that data space objectives are relevant, feasible, and compliant with user expectations and EU standards. Validation II, Thematic Group Validation, encourages collaboration among stakeholders to validate thematic



Figure: 1 Validating Design Principles - Workflow

relevance, identify synergies, and anticipate challenges. *Validation III*, Expert Group Validation, leverages specialized expertise to scrutinize technical feasibility, ensuring adherence to expert and partner feedback. This iterative approach promotes thoroughness, inclusivity, and integration of design principles, thereby enhancing the efficacy and sustainability of data-driven initiatives.

RESULTS AND DISCUSSION

The summarised matrix shown in Table 1 provide insights into various CSAs focusing on different sectors such as agriculture, smart cities, skill mapping, cultural energy, heritage, genomics, environmental sustainability, and language data. Each CSA emphasizes different aspects of business design,



Table: 1 Validating Design Principles for CSAs - Analysis

governance, legal considerations, data interoperability, and data product development. While some CSAs excel in certain areas, such as business and governance principles, they may lack depth in others, like legal considerations or data interoperability. Overall, each CSA requires further refinement and enhancement to comprehensively address all design principles and effectively achieve their objectives.



Abstract



P2P energy trading & market clearing results in a notable decrease in energy costs, with the community paying ~37% less for energy compared to farms that don't use P2P approach. Moreover, during peak hours, dependence on the grid is reduced by ~41.10% and the revenue generated by selling the excess electricity is increased by ~55%, as seen in figure 2a, 2b, and 2c.



Abstract

Incorporation of an Unbalanced Rotating Mass System to Accelerate the Fatigue Testing of Tidal Turbine Blades

Tenis Ranjan Munaweera Thanthirige¹, Michael Flanagan¹, Ciaran Kennedy¹, Jamie Goggins¹, William Finnegan¹

1. Construct Innovate and SFI MaREI Research Centre, Ryan Institute, School of Engineering, University of Galway, H91 TK33, Galway, Ireland

INTRODUCTION

The tidal energy sector is advancing next-generation tidal energy convertors (TECs) to ensure the effective utilising of untapped tidal potential worldwide, offering a promising avenue for generating clean, affordable electricity. However, the industry faces several challenges including the validation of the structural integrity of TECs, prior to their deployment. The main barrier is related to validating the estimated lifespan of these blades. This involves extensive fatigue testing, aligned with industry standards such as DNVGL-ST-0164 and IEC DTS 62600-3, often involving millions of cycles. In this situation, employing servo hydraulic actuators for such testing imposes significant time constraints due to operational limitations.

MATERIALS AND METHODS

The main aim of this study is to explore the effectiveness of using Unbalanced Rotating Mass (URM) system in conducting fatigue testing for next-generation tidal turbine blades and compare the performance with conventional servo hydraulic actuators. In this situation, a 5-meter-long helical-shaped crossflow tidal turbine foil was utilised for fatigue testing, employing a URM system. The URM was attached to one end of the turbine foil, allowing it to induce excitation. This excitation was adjusted to closely align with the foil's first natural frequency, thereby inducing resonance for conducting fatigue cycles.

RESULTS AND DISCUSSION

The findings of the study suggest that the URM system offers several advantages over its traditional counterpart. Notably, it speeds up fatigue life testing, enabling researchers to expedite the structural validation process of the turbine foil, in terms of withstanding fatigue cycles over its operational design life. Additionally, the URM system demonstrates improved reliability and user-friendliness, providing smoother excitation control on the turbine foil during the testing process. These approaches enhance the effectiveness of the testing program while reducing testing duration. Consequently, the utilisation of the URM system effectively accelerates the de-risking process of next-generation tidal turbine systems and promote the rapid development of TECs. However, the URM system may not be suitable for highly rigid tidal turbine blades and requires a mechanism to measure the excitation load on the foil. These deficiencies are considered the primary limitations of using URM systems for fatigue testing of tidal turbine blades. Therefore, integrating a precise mechanism to monitor excitation loads on the blades would enable the utilisation of the URM system for testing small-scale, less stiff tidal turbine blades. In this context, the adoption of this cutting-edge URM technology for structural testing of tidal turbine blades, driving the tidal energy industry transition towards a more sustainable future.



Abstract

GDPR-Compliant Video Search and Retrieval System for Surveillance Data

Shifa, Amna¹, Asghar, Mamoona¹, and Kennedy, Rónán² ¹ School of Computer Science, University of Galway ² School of Law, University of Galway

INTRODUCTION

The widespread deployment of surveillance cameras, responds to the increasing demand for scene investigation, video forensics, and analytics. This necessitates the accurate retrieval of required video shots for post-verification. However, the massive volume of video data (big data) poses a challenge in efficiently filtering the retrieval results. Additionally, surveillance videos often contain sensitive Personally Identifiable Information (PII) about individuals, raising concerns about privacy and data protection. In response to these concerns, European regulatory authorities have enforced the General Data Protection Regulation (GDPR) to safeguard individuals' privacy rights and mitigate security threats. This work aims to provide a multi-layered secure and efficient retrieval mechanism (Figure 1) of desired video frames during investigations, which are stored in encrypted form.

MATERIALS AND METHODS

In the proposed solution, initially, high-level features such as objects and activities within the video will be detected through semantic segmentation employing a Fully Convolutional Network (FCN). Subsequently, the detailed semantic representation of textual input disentangles the textual sentence into contextual words (metadata), namely verbs and nouns, which are then aggregated using the long short-term memory (LSTM) architecture. After that, this metadata will be matched and embedded with global features. Finally, the labelled video will be protected by implementing partial lightweight encryption (PLE) before being stored on storage devices, from where it can be retrieved as needed. With PLE, only feature-of-interest (FoI) will be encrypted, resulting in substantial savings in storage capacity, encryption space ratio (ESR), and latency impact. However, if there is a need to reveal the protected video, authorized persons can decrypt it using the encryption key.



Figure 1: Proposed Multi-layered architecture for efficient retrieval of encrypted videos

CONCLUSION

The proposed solution provides robust GDPR-compliant security features, enabling solution providers to protect videos in a retrievable form without decryption, thereby safeguarding digital and human rights in recorded video data. It is aligned with UN Sustainable Development Goals (SDGs) such as SDG 9: "Industry, Innovation, and Infrastructure" and SDG 11: "Sustainable cities and communities".



Abstract

Gold nanoparticles localised within photoactive covalent organic frameworks as photocatalysts for CO_2 reduction

McCarthy, K.1; González R.G.2; Costa, P.F.3

_{1,2,3} School of Biological and Chemical Sciences, Ryan Institute, University of Galway, University Rd, Galway, H91 TK33, Ireland

Concerning levels of CO_2 in the atmosphere have urged researchers to investigate using CO_2 as a feedstock for carbon-based fuels and value-added chemicals via photocatalytic reduction. Recently, porous materials, such as covalent organic frameworks (COFs), have been explored as working supports for photocatalysts due to their remarkable physical/chemical stability, structural diversity and large surface areas. Furthermore, light-harvesting ability can be enhanced by careful selection of building blocks, while also tuning the bandgap to extend the lifetime of electron-hole pair separation, thus establishing a thermodynamically favourable process.

Hybrid photocatalysts can be formed by incorporating metal nanoparticles (MNPs) into the photoactive COF network, creating an electron "donor-acceptor" type photocatalyst, wherein electrons excited within the framework can be accepted by the MNP to reduce CO₂. MNPs are widely used for catalysis due to their high surface energy and quantum size effects; in particular, gold nanoparticles (AuNPs) are highly selective towards CO₂ reduction. However, aggregation of MNPs can result in gradual loss of catalytic activity, therefore uniformly immobilising them on light-harvesting, porous supports is effective in extending their photocatalytic performance.

In this work, size controlled AuNPs were synthesised *in-situ* into a thiol-functionalised porphyrinperylene COF, resulting in a novel material for the purpose of photocatalytic CO₂ reduction. Thiol groups, in combination with the framework pores, assist in localisation and size control of the AuNPs, resulting in a homogeneous material designed to enhance efficiency and selectivity towards the production of value-added chemicals. This material will be tested for photocatalytic CO₂ reduction, using a sacrificial agent, under visible light irradiation at different temperatures and operating conditions. In particular, a comparison between batch and flow conditions will be evaluated for activity, stability and selectivity and products will be quantified using gas chromatography.



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INNOVATION FOR HEALTH

Oral Presentations



Abstract

Using purine nucleosides as adjuvants to re-sensitize MRSA to β -lactam antibiotics

Nolan AC¹, Zeden MS¹, Kviatkovski I², Campbell C¹, Urwin L³, Corrigan RM³, Gründling A², O'Gara JP¹

- 1. Microbiology, School of Biological and Chemical Sciences, University of Galway, Ireland
- 2. Section of Molecular Microbiology and Medical Research Council Centre for Molecular
- Bacteriology and Infection, Imperial College London, London, United Kingdom
- 3. The Florey Institute, School of Bioscience, University of Sheffield, Sheffield, United Kingdom

INTRODUCTION

Infections caused by antimicrobial resistant (AMR) pathogens are currently on the rise causing significant burden on healthcare systems worldwide. By 2050 it is believed that 10 million deaths will be caused by AMR infections. There are dwindling options for AMR pathogens as most antibiotics are becoming ineffective for treatment of these infections. Using combinations of antibiotics with other antibiotics or non-antibiotic drugs may extend the usefulness of currently used antibiotics and provide some solutions to slow or prevent our slide into a post-antibiotic era. We have discovered that the purine nucleoside guanosine can re-sensitise MRSA to beta-lactam (penicillin-type) antibiotics.

MATERIALS AND METHODS

Antibiotic susceptibility assays were performed with the beta-lactam antibiotic oxacillin and guanosine. MRSA cells grown in a guanosine + oxacillin combination were viewed under confocal microscopy and transmission electron microscopy. Kill curve assays were carried out to determine the efficacy of adding guanosine to oxacillin and measure its effect on cell viability.

RESULTS AND DISCUSSION

Our data reveals that guanosine supplementation can increase beta-lactam efficacy against MRSA. This is shown by increased zones of inhibition around antibiotic discs when MRSA was grown on Mueller Hinton Agar supplemented with guanosine. Further research into the mechanism underpinning this phenomenon identified changes in metabolic pathways within MRSA cells. Transmission electron microscopy analysis revealed that MRSA treated with guanosine and oxacillin were significantly larger than cells treated with oxacillin alone (Figure 1). Furthermore MRSA cells treated with oxacillin and guanosine displayed thinner cell walls and an increased number of septa indicative of aberrant cell division. These data indicate that guanosine disrupts osmotic regulation in MRSA and targets the cell envelope leading to cell division defects. These combined effects highlight the therapeutic potential of purine nucleosides such as guanosine for the improved treatment of MRSA infections.



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FIG 1. Exogenous guanosine increases damage beta-lactam damage to MRSA cells viewed using TEM. (A) Cells were grown in Muller Hinton broth (MH), (B) MH + 200 μ g/ml guanosine (MHG), (C) MH + 1 μ g/ml oxacillin (MHO) and (D) MH + 200 μ g/ml guanosine + 1 μ g/ml oxacillin (MHGO).



Abstract

Towards Optimized Cell Cargo for Encapsulation Devices in Type 1 Diabetes

Trask, L.1, Ward, N.A.1, O'Dwyer, J.2, Duffy, G.D.2, Dolan, E.B.1.

Biomedical Engineering, College of Science and Engineering, University of Galway
 Anatomy and Regenerative Medicine Institute (REMEDI), School of Medicine, College of

Medicine Nursing and Health Sciences, University of Galway

INTRODUCTION

Encapsulation devices are being developed to protect transplanted islets and serve as a bioartificial pancreas in type 1 diabetes (T1D). Despite some success, they have limited long-term viability, in part due to the diffusion barrier they pose which is exacerbated by the foreign body response (FBR)¹. We have previously developed an actuatable soft robotic device to decrease the magnitude of the FBR^{2,3} and are now redesigning it for cell cargo. We aim to determine if these devices containing optimized cell cargo can overcome current challenges.

MATERIALS AND METHODS

The device was redesigned from previously validated configurations^{2,3} to house cell cargo (**Fig 1A**). We investigated if more robust pseudo-islets (PIs) could be generated by co-culture and combination with a suitable carrier. Co-cultured PIs were generated using the INS1E β - and TC1 α -cell lines and stained for insulin and glucagon to identify cell-type. PIs were combined with a macroporous gelatin sponge carrier (SpongostanTM–SF) and stained with DAPI to investigate their distribution. Function was evaluated by insulin secretion at low (3.3mM) and high (16.7mM) glucose concentrations⁴.

RESULTS AND DISCUSSION

We generated co-cultured PIs, however, they formed 'islands' of α -cells rather than proper spherical morphology (**Fig 1B**). We therefore combined β -cell only PIs with SF and demonstrated their 3D integration (**Fig 1C**). The developed PIs were functional with significant increases in insulin secretion in both media and the carrier (**Fig 1D**, *p<0.05). As encapsulation device failure is often due to poor factor transport which is further inhibited by the FBR, the combination of optimized cell cargo with a fibrosis mediating soft-robotic device may help serve as a bioartificial pancreas for T1D.



Figure 1: A) Actuatable soft-robotic device. B) Co-cultured PIs stained by cell type. C) PI distribution in the carrier (SF). D) PI functionality in media (free) and carrier (SF).

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Abstract

DIELECTRIC PROPERTIES OF HUMAN PARATHYROID GLA DIFFERENTIATION OF THYROID AN	ANDS: A POTENTIAL TOOL FOR INTRAOPERATIVE
<u>Amin, B.</u> ^{1,2,3} , Shahzad, A. ⁴ , González-Suárez, A. ^{1,2,3} , Dur Elahi, A. ^{1,2}	nne, E. ^{1,2,3} , Lowery,A. ⁵ , O'Halloran, M. ^{1,2,3} ,
 Llahi, A.^{1/2} ^{1.} Translational Medical Device Lab, Universit ^{2.} Electrical and Electronic Engineering, Universit ^{3.} School of Medicine, University of Ge ^{4.} Centre for Systems Modelling and Quantitat and Systems Research, University of Birm ⁵Discipline of Surgery, Lambe Institute for Translational Dielectric properties of parathyroid glands could be us intraoperative identification of parathyroid glands. I parathyroid gland would aid the preservation of th incidence of post-surgical hypoparathyroidism after th identification of accidentally removed parathyroid glar transplantation process, which aims to save the function of the incidence of post-surgical function of the same transplantation process. 	y of Galway, H91 TK33 Galway, Ireland sity of Galway, H91 TK33 Galway, Ireland alway, H91 TK33 Galway, Ireland ive Biomedicine, Institute of Metabolism ningham, Birmingham B15 2TT, U.K. I Research, University of Galway, Ireland sed as potential information by surgeons for the Early confirmation that the tissue is indeed a e tissue and has the potential to reduce the yroid and/or parathyroid surgery. Currently, the nds relies on intraoperative frozen biopsy, which dentifying the glands hinders the timely auto- ction of parathyroid glands that could not be
and reliably identify parathyroid glands during thyro dielectric properties of the <i>ex vivo</i> dielectric properties	id surgeries. This study aimed to evaluate the s of human parathyroid glands in the microwave
the dielectric properties of the human parathyroid gla parathyroid glands were acquired from a total of nir ethical approval from the Clinical Research Ethics Co	ands for a frequency range of $0.5 - 8.5$ GHz. The patients ($N = 9$) with informed consent and monitize Galway University Hospitals Ireland
Eight out of nine patients were diagnosed with parat diagnosed with nodular hyperplasia ($N = 1$). The mea human parathyroid gland samples. The relative perr conductivity ranged from 0.9 – 9 S/m over the frequ insights into the dielectric properties of human parath the development of microwave-based techniques	hyroid adenoma ($N = 8$) while one patient was asurements were conducted on freshly excised mittivity values ranged from 42 – 57, and the uency range of 0.5 – 8.5 GHz (Figure 1). These hyroid glands have the potential to be used for for non-invasive detection, localisation, and
functional assessment of parathyroid glands, which parathyroid-related disorders, such as hyperparathyro	will lead to improved clinical management of bidism.
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40 L	0 2 4 6 8 10 frequency [GHz]





Abstract

VISCOPLASTIC BEHAVIOUR OF FIBRIN-RICH BLOOD CLOTS
Bein Snee, K. ¹ , McCarthy, R. ² , McGarry, P. ¹
1. Biomedical Engineering, University of Galway, Ireland
2. Cerenovus, Ireland

INTRODUCTION

During aspiration thrombectomy for ischemic stroke, a catheter is used to apply suction pressure to a clot in order remove it from the cerebral vessel. Various approaches have been proposed to increase clot ingestion efficacy, especially of tough (fibrin-rich) clots [1]. While the viscoelastic properties of clots have been established previously, the viscoplastic permanent deformation of clots has not been investigated. A fundamental understanding of such inelastic behaviour may play a key role in the design of next-generation thrombectomy devices.

MATERIALS AND METHODS

Fibrin-rich clots (5% hematocrit) were fabricated as described previously [2]. A loading platen was used to apply an axial compression to two sets of cylindrical clots of initial undeformed height h_0 , reducing the height h of the clots to $(h_{min}/h_0) = 0.4$ and $(h_{min}/h_0) = 0.2$, respectively. The loading platen was then instantaneously removed, and the recovery of h was monitored for one hour. A third set of clots was held at $(h_{min}/h_0) = 0.4$ for one minute before the platen was retracted. A fourth set of clots was subjected to aspiration at an applied pressure of -80 kPa for 5 minutes. We developed a novel composition-dependent anisotropic hyperelastic-viscoplastic constitutive law to replicate our experimental results [2]. Plasticity is implemented through permanent fibre alignment and changes in density in the blood clot's fibrin network.

RESULTS AND DISCUSSION

An increase in the applied compressive strain magnitude and duration result in an increase in permanent deformation (Figure 1A, 1B). Compressed clots do not return to their pre-test configuration, confirming and quantifying for the first time, viscoplastic behaviour (Figure 1C). Permanent deformation of partially ingested clots is observed after aspiration (Figure 1D). Our anisotropic hyperelastic-viscoplastic finite element model can accurately predict our experimental findings (Figure 1B, 1E).



Figure 1: Increased compressive strain magnitude (A) and loading duration (B) lead to increasing permanent deformation of clots; Permanent deformation following compression (C) and partial aspiration (D); Novel viscoplastic simulation of permanent deformation during partial aspiration (E).

References and Acknowledgements

1. Munoz et al, Interv Neuroradiol, 29:450-458, 2023; 2. Fereidoonnezhad et al, Biomech, 130: p. 110865, 2022 Funding provided by Irish Research Council (EPSPG/2022/379) and Enterprise Partner Cerenovus (Neuravi Ltd.).



Abstract

Formation 3D super-resolution nanosensitive images of biological objects	
Alexandrov, S, McAuley, R., Dey, R., Arangath, A., Zhou, Y., and Leahy, M.	
School of Natural Sciences, Tissue Optics and Microcirculation Imaging (TOMI) group	

INTRODUCTION

Visualization of nanoscale structural changes in biological samples for early detection of different pathologies poses a significant challenge. The fundamental resolution limit was overcome and in 2014 Nobel prize was given for invention of super-resolution microscopy. However, this microscopy largely requires labelling, is limited to superficial 2D imaging, and is generally not suitable for in vivo applications to study organisms in natural conditions. Furthermore, it is becoming evident that 2D biology often does not translate into the real 3D situation. Optical coherence tomography (OCT) facilitates 3D label-free, depth resolved structural and functional imaging of living tissues. However, the structural sensitivity and resolution of intensity-based OCT imaging are fundamentally limited to microscale. Here, we present the label-free approach for super-resolution 2D and 3D imaging and quantitative sensing of highly scattering objects, including humans in vivo.

METHODS

We developed the spectral encoding of spatial frequency (SESF) approach for label free visualization of the sub-wavelength structure with nanosensitivity to structural alterations. This approach is based on collection of high spatial frequencies of the object by using broadband light sources and reconstruction of the axial spatial frequency profiles at each point within the image. Then the image can be formed as a colour map of some informative parameters of these profiles, for example as a colour map of the dominant structure, or correlation between profiles, etc. The SESF approach has been adapted for label free 3D *in vivo* imaging of highly scattering media using OCT; we call this technique nanosensitive OCT (nsOCT). In our talk we will describe the principles of the SESF approach and nsOCT, and demonstrate different applications which show advantages of these novel technique in comparison with existing methods.

RESULTS AND DISCUSSION

One example application of the SESF approach for detection of tumour regions is presented in Fig. 1. It is impossible to detect the structural changes between normal and pathological tissue in conventional OCT images in Fig. 1 left, but such changes can be clearly visualized in nsOCT images in the right. Colours in the nsOCT image of tumour tissue are shifted to red, suggesting increase of the dominant size of nanostructure.



Figure 1: Conventional OCT (on the left) and nsOCT (on the right) images of the normal (top) and tumour (bottom) tissue.



An Agent-Based Deep Learning Computational Framework For The Simulation Of Mechanosensitive Tumour Growth
Senthilkumar, I. (1, 2, 3), Howley E. (1, 2), McEvoy E. (3)
 School of Computer Science, University of Galway, Ireland Data Science Institute, University of Galway, Ireland Discipline of Biomedical Engineering, University of Galway, Ireland
 INTRODUCTION Tumour growth is influenced by mechanical interactions between cells and the surrounding extracellular matrix (ECM). We have developed a novel hydro-mechanical model and integrated it with an agent-based (AB) framework with a novel artificial intelligence-accelerated (AI) finite element (FE) solver, to simulate mechanosensitive spheroid growth. MATERIALS AND METHODS Cell volume is regulated by a competition between hydrostatic pressure arising from active cell stress and external loading, and osmotic pressure arising from ion fluxes [1] (Fig. 1A), while cell growth arises from biomolecular synthesis. Cells divide when a mitotic volume checkpoint V_{crit} is surpassed (Fig. 1B). We integrate our novel cell growth model with PhysiCell [2], an AB modelling framework. Synthetic training data is generated using a novel data collection framework for FE software Abagus, allowing for FE predictions 1.5Mx faster than CPU-based FE (Fig. 1C).
RESULTS AND DISCUSSION Cell confinement elevates hydrostatic pressure and decreases cell volume due to fluid loss, restricting proliferation by preventing cells from surpassing the mitotic checkpoint. Our integrated AB-AI-FE framework for 4T1 spheroid growth simulations indicate tumour size reduces with increasing matrix stiffness aligning with our experimental data (Fig. 1D) [3]. Simulation of multicellular proliferation using our computationally efficient AB-AI-FE model provides unique insight into the evolution of macro-scale tissue behaviour and mechanosensitive growth, with broad applications to patient-specific cancer diagnosis.

Confinement Stress (Pa)

4000 8000 12000 Number of Nodes

Figure 1: (A) Cells grow from biomass synthesis; (B) Stress constrains mitosis; (C) The AI-FE framework is 1.5Mx faster than CPU operations. (E, F) 4T1 Spheroid size decreases with

CPU Runtime
 GPU Runtime
 NN Runtime

-0.5

-0.25

Radial Stress (kPa)

0 2250

2750

Cell Volume (µm³)

3250

С

(s) 1e1 CPU Time

1e-1-GPU

5 1e-3 NN



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increased matrix stiffness due to matrix feedback.

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cycle progression



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Mechanosensitive Role of Osteocytes in Governing Osteoclast Resorption in Postmenopausal Osteoporosis: Insights from an Advanced 3D In Vitro Model

Naqvi¹, S.M., O'Brien¹, T., Martin², R., Verbruggen¹, A, and McNamara¹, L.

1. Mechanobiology and Medical Device Research Group (MMDRG), University of Galway, Ireland INTRODUCTION: Postmenopausal osteoporosis, characterized by severe bone loss due to estrogen

deficiency, also entails fundamental changes in bone tissue composition associated with changes in the mechanobiological response ^[1-4]. Previously, we developed a simplified 3D postmenopausal model of osteocyte differentiation, which revealed changes in mineralization and pro-osteoclastogenic paracrine signalling by osteoblast derived osteocytes during estrogen deficiency^[5]. Despite advancing our understanding of the disease, this study did not fully recapitulate the in vivo multicellular environment, which governs osteoclast activity and associated bone loss during osteoporosis, or the biophysical environment. Here our objectives were to (1) incorporate a multicellular niche within a suitable matrix, (2) apply exogenous mechanical loading to the constructs, and (3) investigate osteoclastogenesis under estrogen withdrawal conditions (mimetic of postmenopausal osteoporosis).

MATERIALS AND METHODS: MC3T3 osteoblast-like cells and OCY454 osteocyte-like cells were pretreated with 17 β -Estradiol prior to encapsulation in Gelatin-nHA hydrogels that were enzymatically crosslinked with microbial transglutaminase. These constructs were then cultured for 21 days in osteogenic media under (1) continued estrogen supplementation (E) or (2) estrogen withdrawal (EW). After 21 days in culture, RAW264.7 osteoclast precursors encapsulated in Gelatin-nHA were layered on top of these mineralised constructs and cultured for a further 14 days in standard growth media. Concurrently, we applied compression (~0.5% strain at 1 Hz) and perfusion (~1.2 mL/min, 1 Hz) using a custom developed bioreactor (VizStim). Static groups served as controls.

RESULTS AND DISCUSSION: Our advanced 3D model was shown to recapitulate osteoclastogenesis and mineralisation. By day 7, all groups had multinucleated and TRAP positive cells (FIG 1A, 1B). Estrogen deficient constructs had significantly higher osteoclastogenic gene expression at day 7 (OSCAR) and day 14 (CTSK) compared to continued estrogen supplementation (FIG 1C, 1D). Mineral deposition was confirmed in all groups by von kossa staining and micro-CT (FIG 1E, 1F). This model was then applied to study osteocyte regulation of osteoclasts under mechanical stimulation and estrogen deficiency. Mechanically stimulated and estrogen deficient constructs had significantly lower ALP activity and calcium content at day 7, continued estrogen supplementation (FIG 1G, 1H). We propose that reduced mineralisation in multicellular constructs was related to the activation of osteoclast resorption.



Figure 1: TRAP (A) and H&E (B) staining; TRAP-positive cells (highlighted by yellow arrows). Gene expression for OSCAR (C) and CTSK (D). Von Kossa staining (E) and micro-CT (F). ALP activity (G) and calcium content (H).

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Abstract

INVESTIGATING THE EFFECTS OF INTERMITTENT ACTUATION ON MACROPHAGE POLARISATION IN
VITRO

Shokrani, P.¹, Ward, N. A¹., Prendeville, H¹., Duffy, G. P.²., Dolan, E.B¹.

1. Biomedical Engineering, College of Science and Engineering, University of Galway

2. Anatomy and Regenerative Medicine Institute (REMEDI), School of Medicine, University of

Galway

INTRODUCTION

The foreign body response (FBR) is a complex cascade of inflammatory events that is initiated in response to medical implants. The FBR can form a fibrous capsule (FC) around the implant, leading to its failure^{1,2,3}. Macrophages are key drivers in the FBR and can modulate inflammation and healing by polarisation into either pro- or anti-inflammatory phenotypes^{4,5}. Strain and fluid flow have been shown to alter macrophage phenotypes^{6,7}. Our group has shown that mechanical actuation of implantable reservoirs can modulate the FBR and reduce the thickness of the FC in both rat¹ and mouse⁸ models. Interestingly, no significant difference was seen in the numerical density of CD68-stained macrophages at 14 days¹. However, little is known about the immunomodulatory mechanisms of actuation. This work aims to examine the effects of actuation on polarisation of M1 macrophage-like THP-1 cells.

MATERIALS AND METHODS

Human leukemia monocytic cells (THP-1s) were differentiated into M0 macrophage-like cells using 100 ng/mL Phorbol-12-myristate-13-acetate (PMA), and morphology was assessed using light microscopy. The cells were then polarised into M1 phenotype using Interferon-gamma (IFN- γ) and Lipopolysaccharide (LPS) at three different ratios of LPS: IFN— γ (1:10, 10:1, and 10:10 ng/mL) for 24 hours. Flow cytometry using CD86 (M1 marker) and CD206 (M2 marker) was used to confirm the polarisation.

RESULTS AND DISCUSSION

PMA treatment causes THP-1s morphology to change from round to amoeboid shape, with increased cell size, characteristics of M0 macrophage-like cells (Fig1.a). M1 polarisation using the 10:1 ng/mL ratio was confirmed with flow cytometry by a significant CD86 upregulation (p<0.005) compared to control and significantly lower CD206 expression compared to the other two ratios (p<0.05) (Fig 1. b). Ongoing experiments are optimising the seeding densities of M1 macrophage-like cells on actuatable reservoirs before determining the immunomodulatory effect of actuation. This model aims to give a better insight into the role of actuation in modulating the macrophage response.



Figure 1. a) Light Microscopy showing morphology change, b) flow cytometry of CD86 and CD206 (MFI: mean fluorescence intensity)

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Abstract

A replenishable, therapeutic implant for the treatment of ovarian cancer

Sheedy, A.M.^{1, 2, 3, 4}, Shetty. M^{3, 4}, Weis. A^{3, 4} Bendzick. L^{3, 4}, Ni. Z^{3, 4}, Geller. M.A³, Miller. J.S, Felices, M^{3, 4}, Dolan, E.B^{1, 2},

¹ Biomedical Engineering, School of Engineering, College of Science and Engineering, University of Galway, Ireland. ² CÚRAM, Centre for Research in Medical Devices, University of Galway, Galway, Ireland. ³ Masonic Cancer Center, University of Minnesota, Minneapolis, MN 55455, USA, ⁴ University of Minnesota, Department of Medicine, Minneapolis, MN 55455, USA

INTRODUCTION

Ovarian cancer is a lethal malignancy with 5-year survival rates of <50%¹. Cell immunotherapy, using expanded Natural Killer cells (eNKc), is a promising new treatment². However, delivery of eNKc to the intraperitoneal (IP) space has proven difficult, with administration of such confined to clinical trials. Multiple clinical trials^{3,4,5}, and follow-up studies⁶, have shown that chemotherapy delivered via repurposed IP catheters significantly extended the median survival rate compared to gold standard IV delivery (65.5 vs 49.7 months)⁵. Interestingly, in that study only 42% of patients completed the recommended 6 rounds of IP treatment⁵. Low completion rate attributed to patient discomfort, infections, blockages and other catheter-related issues⁵. Here, we deliver eNKc immunotherapy to the IP space in mice through a specifically designed, replenishable therapeutic implant and compare to IP injection.

MATERIALS AND METHODS

Our study compared the delivery of therapy (eNKc + interleukin (IL)-15) through our implant vs gold standard IP injection. NOD-scid-gamma (NSG) mice received our implant on day -14. Both groups received human ovarian cancer cell line, DlucOVCAR8, on day-3 and animals were irradiated on day-1. Implant and gold standard IP groups received the therapy regimen ($5x10^6$ eNKc 1x/week and 0.98ng IL-15 3x/week) or control (sterile saline 3x/week) for 6 weeks. Tumor burden was monitored weekly with bioluminescence imaging.

RESULTS AND DISCUSSION

Therapy (eNKc+IL-15) delivered through our implant or via IP injection controlled the tumour burden over the study period (Figure 1). This was significantly better than saline delivered by both methods at every time-point, validating our model and in agreement with Geller et. al., 2013⁷. Therapy delivered through our implant significantly improved the tumour burden compared to IP injection at 35 (p=0.1) and 42 days (p=0.016).



Gold Standard Device **IP** Injection eNK + Saline eNK + Saline Control □ IL-15 **Figure 1:** Area under Normalised Radiance (p/s) curve AUC denoting overall therapeutic functional effect mapped over study duration. Statistical comparisons are saline control: G.S. IP vs Device, eNK + IL-15: G.S. IP vs Device, G.S. IP: Saline control vs eNK + IL-15, and Device: Saline control vs eNK + IL-15. There is no significant difference between saline control: G.S. IP vs Device at any time points. From D35 Device maintains tumor burden significantly better than G.S. IP Injection in eNK + IL-15, D35 (42.99± 26.27 vs 193.54±138.18) and D42 (52.16±29.98 vs 334.58±155.55).

CONCLUSION

Our novel implant can deliver therapy to the IP space in an ovarian cancer setting. It maintained tumor burden for 42 days, significantly better than the current gold standard on day 35 and 42. This study provides a step closer to clinical translation of the implant, which could provide better clinical outcomes for ovarian cancer patients.

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Abstract

Metabolic reprogramming and altered cell envelope characteristics in a pentose phosphate pathway mutant increases MRSA resistance to β-lactam antibiotics

Zeden, M.S.¹^{*}, Gallagher, L.A.₁, Bueno, E.₂, Nolan, A.C.₁, Ahn, J.₃, Shinde, D.₃, Razvi, F.₃, Sladek, M.₃, Burke, Ó.₁, O'Neill, E.₄, Fey, P.D.₃, Cava, F.₂, Thomas, V.C.₃, O'Gara, J.P. ^{*}

- 1. School of Biological and Chemical Sciences, O'Gara & Zeden research groups, College of Science and Engineering, University of Galway, Ireland
- 2. Department of Molecular Biology, Umeå University, MIMS—Laboratory for Molecular Infection Medicine Sweden, Umeå, Sweden
- 3. Department of Pathology and Microbiology, University of Nebraska Medical Center, Omaha, Nebraska, United States of America
- 4. Department of Clinical Microbiology, Royal College of Surgeons in Ireland, Dublin, Ireland

INTRODUCTION

Antibiotics have long represented a successful form of therapy in medicine. However, experts predict that antimicrobial resistance (AMR) due to infections by so-called "superbugs" could kill 10 million people annually by 2050. Identification and exploitation of new targets to improve the treatment options for AMR infections is a necessity. Central metabolic pathways control virulence and antibiotic resistance, and constitute potential targets for antibacterial drugs. In *Staphylococcus aureus* the role of the pentose phosphate pathway (PPP) remains largely unexplored.

MATERIALS AND METHODS

A Nebraska Transposon mutant of the 6-phosphogluconolactonase gene *pgl*, which encodes for the only non-essential enzyme in the oxidative phase of the PPP in MRSA strain JE2 was utilised. Carbon tracing and metabolomics was used to trace flux of carbon to glycolysis versus PPP. Transmission Electron Microscopy and Confocal Microscopy (Fig.1) was used to investigate the morphology of the cells with and without oxacillin. Levels of lipoteichoic acids (LTAs), wall teichoic acids (WTAs) and peptidoglycan crosslinking were examined. The cell surface charge and antibiotic susceptibility profile of the strains were determined.

RESULTS AND DISCUSSION

The *pgl* mutant had significantly increased MRSA resistance to β -lactam antibiotics, particularly in chemically defined media with physiologically-relevant concentrations of glucose. Metabolomic analysis revealed extensive metabolic reprogramming in the *pgl* mutant. Morphologically, *pgl* mutant cells were smaller than WT with a thicker cell wall and ruffled surface when grown in oxacillin. The *pgl* mutation reduced resistance to Congo Red, sulfamethoxazole, but increased resistance to targocil, fosfomycin and vancomycin. LTAs were significantly reduced in *pgl*, which may limit cell lysis, while the surface charge of *pgl* cells was significantly more positive. Collectively these data show that reduced levels of LTAs and oxacillin-induced lysis (Fig.1) combined with an increase in cell surface positive charge are accompanied by significantly increased oxacillin resistance in MRSA *pgl* mutant.

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Figure 1: Representative microscopic images of JE2, *pgl* and *pgl* complemented cells grown in Chemically Defined Medium with Glucose supplemented with oxacillin 0.05 μ g/ml and labelled with vancomycin BODIPY FL, which binds to the terminal d-ala-d-ala in the peptidoglycan stem peptide (green, top panel) or WGA Alexa Fluor 594, which binds to GlcNAc and other sugars in the cell envelope (red, bottom panel).



Abstract

A MULTISCALE FRAMEWORK FOR THE GROWTH AND REMODELLING OF CONTRACTILE TISSUE

Thomas Hayes(1,2), Ankita Pramanick (2), Andrew Daly (2), Giuseppe Zurlo (1), Eóin McEvoy(2)

- 1. School of Mathematical and Statistical Sciences, University of Galway, Ireland;
- 2. Discipline of Biomedical Engineering, University of Galway, Ireland.

INTRODUCTION

The growth of contractile tissue depends on a complex interplay between active cell tension, mass transport, and assembly/disassembly processes. Complex shape changes arising during morphogenesis can be explored through advanced bioprinting platforms, facilitating the precise positioning of cells and extracellular matrix [1] to analyse subsequent remodelling. To understand the biomechanisms underlying dynamic morphological evolution of contractile tissues more deeply, we propose a novel computational model that considers the thermodynamics of cytoskeletal growth and force generation that guide tissue-level remodelling.

METHODS

<u>**Cell Level:**</u> Muscle and non-muscle cells generate active forces through the remodelling and force generation of contractile actomyosin fibers. These processes are, in turn, highly sensitive to cytoskeletal stress (σ_f), stretch (λ), and strain rate [2]. Radial growth (λ_{rr}^g) of these contractile fibers can be described by:

$$\lambda_{\rm rr}^{\rm g} = \left[\frac{1 - \lambda_{\rm rr}^{\rm g} \lambda_{\rm zz}^{\rm g}}{\pi \lambda_{\rm zz}^{\rm g}}\right] \exp\left\{-\frac{\lambda_{\rm zz}^{\rm g}(\mu_b - \mu_u)}{k_B T}\right\},\,$$

where $\mu_b(\sigma_f)$ and $\mu_u(C)$ are the enthalpies of the assembled and unassembled fiber proteins, respectively.

Tissue Level: The active framework is combined in parallel with a passive anisotropic hyperelastic model [3,4]. The combined active and passive framework was implemented using user-defined material subroutines within the Finite Element (FE) software Abaqus. The developed computational model was applied to predict the biomechanical behaviour of contractile cells and tissue. The framework is validated by bioprinting contractile tissues using a fibroblast-collagen bioink, with construct evolution analysed over 14 days.

RESULTS



Radial growth increases when strain reduces, with the most significant growth occurring under compressive strains. The influence of strain on radial growth is accentuated as the activation signal (C) intensifies (Fig. 1A). A competitive relationship exists between radial (λ_{rr}^{g}) and axial (λ_{zz}^{g}) growth, creating an inverse relation between the two. Intersecting at a strain (ε) of 0.35, where growth ceases in both directions ($\lambda_{rr}^{g} = \lambda_{zz}^{g} = 1$) (Fig. 1B). Bioprinted circular patterns contract over a two-week period (Fig. 1C). Simulations of this geometry reveal how active stress causes this morphology evolution (Fig 1D) and successfully predict experimental

outcomes (Fig 1E). A parameter sweep of the simulated geometry indicated cell concentration (f_0) promotes diameter shrinkage, which is mitigated by increased tissue stiffness.

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Device Deployment and the Onset of Structural Valve Degeneration: Simulation of Transcatheter Aortic Valve Implantation In Vitro

Boxwell, S¹, Armfield, D², Hickey, W³, Cook, S³, Kelly, P³, Cardiff, P², McNamara, L²

¹Mechanobiology and Medical Device Research Group, Biomedical Engineering, College of Science and Engineering, University of Galway, Galway

²School of Mechanical and Materials Engineering, University College Dublin, Dublin ³Structural Heart, Boston Scientific Corporation, Galway

INTRODUCTION

Transcatheter aortic valve implants (TAVI) are minimally invasive medical devices for treatment of aortic stenosis. TAVI oversizing and eccentric deployment can result in leaflet distortion, altered kinematics and unphysiological blood flow, which may predispose these devices to structural valve degeneration (SVD) and early failure [1-4]. The mechanisms of SVD are linked to mechanical and haemodynamic stresses [1,5-7]. Computational approaches, including finite element (FE) analysis and computational fluid dynamics (CFD), have been applied to provide an insight into the onset of SVD in vivo [2-6]. However, the relationship between TAVI deployment, including oversizing and eccentricity, and the onset of SVD, remains poorly understood. The objectives of this study are to (1) develop FE and CFD models of a self-expanding TAVI device, (2) validate against in vitro testing, and (3) investigate the onset of SVD with

device oversizing and eccentricity.

METHODS

FE models of the ACURATE Prime were developed using Abagus/Explicit, with representative material properties. The FE framework (Fig. 1A) simulated crimping (1), deployment (2-3) and the cardiac cycle. Peak systolic configurations were extracted and used to develop CFD simulations in OpenFOAM. We validate models against parameters relating to clinical device performance (geometric orifice area, transvalvular gradient, pinwheeling and stent deflection) from in vitro testing conducted in a ViVitro pulse duplicator. Following validation, we deploy the device within aortic annuli with clinically-relevant oversizing and eccentricity indices, to examine the impact of deployment on device biomechanics.



RESULTS AND DISCUSSION

Figure 1: (A) Simulation of (1) Crimping and (2-3) Deployment of TAVI Device, (B1) In Vitro and In Silico Circular and Elliptical Deployment, (B2) TAVI Stent Deflection showing Von Mises Stress

Our computational models show excellent ^L

alignment with in vitro data (Fig 1B) [geometric orifice area (5.21cm² vs 4.75cm²), pinwheeling (8.50% vs 5.97%) and stent deflection (1.92mm vs 1.763±0.275mm)]. Peak leaflet von Mises stress (2.58 MPa vs. 3.36 MPa) and pinwheeling (8.50% vs 6.20%) decreased when the device was oversized relative to the annulus. Thus, TAVI oversizing (up to 20%) may reduce leaflet stress in regions prone to device failure in vivo [1]. In highly elliptical annuli, coaptation mismatch and severe pinwheeling was observed, previously correlated with premature tissue degradation [8], and were accompanied by increased von Mises stress. Our findings align with previously published studies [3,4,5], which suggests that TAVI elliptical deployment alters device kinematics, which may impact device durability in vivo.

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OLLSCOIL NA GAILLIMHE UNIVERSITY OF GALWAY

Coláiste na hEolaíochta & na hInnealtoireachta College of Science & Engineering

SUSTAINABLE FUTURES

Oral Presentations



Abstract

Modelling nutrient emissions into waterbodies caused by various land-use	
<u>Alighanbari, s.a</u> , Styles, d.s ₂ . <u>Clifford, e.c</u> 1	
¹ School of Engineering, Civil Engineering and Ryan Institute, University of Galway, Galway, Ireland,	
H91 HX31.	
² School of Biological & Chemical Sciences, University of Galway, Galway, Ireland, H91 HX31	

Land use changes caused by agriculture, urban development, industrial activities and forestry can put significant pressure on the environment. Evidence-based strategies are needed to ensure that land use aligns with environmental, societal and climate change mitigation goals. Ireland's agriculture, forestry & other land use (AFOLU) sector is responsible for over 40% of national greenhouse gas (GHG) emissions as well as being a significant contributor to water quality challenges. However, the sector is vital in terms of food production, rural economies and in sustaining communities. Approaches which enable rural communities to thrive while delivering more sustainable land uses supporting, *inter alia*, improved water quality, are required.

There are various models available internationally (e.g. SPARROW, SWAT, MARINA, etc.) which can be used to model the impacts of various anthropogenic and natural activities on water quality. In Ireland, for example, the SLAM model allows us to categorize and estimate nitrogen and phosphorus loss from key sources, including forestry, agriculture, wastewater discharges and urban areas. To date this has not yet been fully linked with land use models such as GOBLIN. GOBLIN is a high-resolution integrated biophysical land use model designed for Ireland's AFOLU sector and has been used to explore prospective land use scenarios compatible with Ireland's commitment to achieve climate neutrality by 2050. However, the linkages between land use change and water quality impacts have yet to be sufficiently modelled.

This study focuses on integrating water quality modelling at a relatively small scale (sub-catchment and catchment) into existing land use models (with a focus on GOBLIN). The study will leverage previous work to improve nutrient loss modelling, nutrient transport modelling and enable land use scenario modelling. Ultimately, this will support integrated modelling to provide rigorous multidimensional assessment of land use strategies.

Key words: land use, nutrient loss modelling, water quality modelling



Abstract

Development of a decision support tool for bridge maintenance based on communities' accessibility.
<u>Fenerich, A. T₁, Lydon, M₁., Vega, A.₂.</u>
1. School of Engineering, University of Galway
2. School of Business, Atlantic Technological University

INTRODUCTION

The decision-making process for prioritising bridge maintenance interventions is a complex task, influenced by numerous factors including the bridge's lifespan, operational characteristics, environmental considerations, and potential consequences of infrastructure unavailability for local communities. This paper addresses the need for a decision support tool to aid bridge owners in prioritising critical bridges, particularly in the context of extensive global maintenance backlogs and limited budgets.

MATERIALS AND METHODS

The proposed tool incorporates the community vulnerability, evaluated by the loss of accessibility effect of bridge failure to essential services. This metric is calculated taking account the street network data, travel time matrix and demographic data on population. Additionally, primary schools and healthcare opportunities data in and around potentially affected areas are included in the evaluation. Once the loss of accessibility is calculated for each region, the criticality of each bridge can be defined and incorporated to the maintenance decision process (Fig. 1). The proposed method in this study relies on the additive method for criteria aggregation and bridge evaluation, with the weights for each criterion set by a bridge asset management expert during elicitation process. Furthermore, a portfolio selection method is applied to ensure compatibility with budgetary constraints.







Coláiste na hEolaíochta & na hInnealtóireachta College of Science & Engineering

RESULTS AND DISCUSSION

The developed approach is not only theoretically robust but also practical for guiding decisionmakers in identifying critical bridges for prioritised maintenance that accounts for broader implications of bridge failures on local communities. The outcomes are expected to facilitate informed decision-making processes for bridge owners, offering an effective solution for optimising resource allocation in the face of limited budgets and growing maintenance backlogs. To illustrate the applicability of the proposed method, ongoing and future efforts involve identifying a suitable case study area in Ireland.

Acknowledgement

This research is part of the EMBRACE-Mobility project, funded by Science Foundation Ireland, under the Sustainable Communities, National Challenge Fund.



Coláiste na hEolaíochta & na hInnealtóireachta College of Science & Engineering

College of Science and Engineering, Research and Innovation Day 2024

Abstract

Empowering citizens toward sustainable food practices: a systematic scoping review of tools and interventions

Olweean, N.1, , Surendran, A.2, Kelly, C.3, Styles, D.1, McArdle, R.4, Mullen, A.1

1. School of Biological and Chemical Sciences, Ryan Institute, College of Science & Engineering

2. School of Psychology, J.E. Cairnes School of Business & Economics

3. School of Health Sciences, Promotion Research Centre, College of Medicine, Nursing and Health Sciences

4. Department of Geography, University College Dublin

INTRODUCTION: Food systems are responsible for one-third of annual greenhouse gas emissions (Crippa et al., 2021), immense biodiversity loss, and environmental pollution, while contributing to hunger and obesity by failing to provide healthy, affordable food for all. The case for food systems transformation is irrefutable and policy from 'farm to fork' has been criticised for its skewed focus on food production. We argue that tools and interventions helping citizens adopt sustainable food practices (SFP) can play a key role in achieving sustainable food system transformation—from 'fork to farm'—which must include bottom-up societal changes and societal buy-in as well as technological advances (Barrett et al., 2020) to be successful. We systematically scope the literature to present the available evidence-based, citizen-centred interventions for SFP.

MATERIALS AND METHODS: The PRISMA-ScR extension protocol (Tricco et al., 2018) was used to identify existing interventions aimed at promoting attitude and/or behaviour change in citizens toward SFP. Search terms were developed with input from an interdisciplinary team of authors. We searched Scopus, Web of Science, and GreenFILE for studies published between 2019, when the landmark EAT-Lancet report on human and planetary health (Willet et al., 2019) was launched, and the day the search was completed (February 29, 2024).

RESULTS AND DISCUSSION: Our search returned 19,410 records, with 17,042 removed (7,236 duplicates and 9,806 not relevant in topic) during initial screening, leaving 2,368 selected for further screening. Examples of variables for data extraction include: location; participant characteristics; setting; study design; food themes (e.g. food choice, food type); intervention mechanism; measured outcomes; and findings. Preliminary results indicate that participants tend to be located in developed countries and part of distinct groups (e.g. students), interventions focus on food choice, food waste, and willingness to act, and outcomes include changes in knowledge, attitudes, and behaviour. Screening is ongoing and will be completed by May 2024.

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Abstract

A systematic review of the impact of climate change on residential buildings performance from an occupant-centric perspective

Reis, D.V.A.^{1, 3}, Loomans, M.G.L.C.², Hajdukiewicz, M.^{1, 2, 3, 4}.

College of Science & Engineering and Ryan Institute, University of Galway, Galway, Ireland
 Department of the Built Environment, Eindhoven University of Technology, The Netherlands
 Construct Innovate, University of Galway, Galway, Ireland
 MaREI Centre, University of Galway, Galway, Ireland

INTRODUCTION

Climate change has profound impacts on the design and operation of residential buildings. The context of progressively warmer summers and increasingly frequent heatwave events not only intensifies the risks of overheating, but also impacts building energy consumption and indoor environmental quality. Europe faces a challenge of providing affordable, high-quality housing for growing populations, while dealing with limited energy sources and the results of changing climate. This drives the need for reliable methods to predict future weather scenarios and their impact on buildings, while appropriately accounting for occupants in the performance assessment. Within this scope, the systematic literature review aims to investigate methodologies and metrics for assessing performance of dwellings under future climate scenarios, including health and wellbeing of building occupants.

MATERIALS AND METHODS

The research considered the PRISMA 2020 approach to identify the current literature on dwelling performance under future weather scenarios. The Mendeley Reference manager and the ASReview Lab tools were used to support screening of articles retrieved from the database search (Fig. 1). The eligible papers were filtered by location and sorted by relevance and quality criteria, to make the final selection of research studies included in this review.



Figure 1: Methodology of the systematic review.

RESULTS AND DISCUSSION

The results of this review indicate the use of future climate models in building simulation tools to project building performance for the changing climate. Thermal and energy-related indices are among the most researched topics, with a preferred focus on assessing overheating risks and heating and cooling demands. On the other hand, the review identified a research gap in the indoor air quality and occupant modelling for future climate scenarios. Despite the complexity and uncertainty surrounding the prediction of building performance in future weather conditions, the computational simulation and the application of uncertainty/sensitivity analysis can provide promising results for occupant-centric building performance in changing climate.



Abstract

Innovative Approaches to Green Hydrogen Production: Alkaline/Saline Seawater Electrolysis Riaz, Muhammad Sohail¹ and Farras, Pau¹

1. School of Biological and Chemical Sciences, Chemlight Group

muhammad.sohail@universityofgalway.ie, Pau.farras@universityofgalway.ie

INTRODUCTION

Saline or low-grade water electrolysis emerges as a promising strategy for addressing the demand for greener hydrogen production. The development of noncritical raw materials-based electrocatalysts is pivotal^[1]. Transitioning to industrial-level applications requires urgently developing scalable strategies for creating these electrocatalysts ^[2]. Our research focuses on advancing the polyol-mediated synthesis of NiFe-based chalcogen systems ^[3], aiming to contribute to future sustainability by enabling efficient hydrogen production.

MATERIALS AND METHODS

In pursuit of our objective, we adopt a polyol-assisted synthesis approach, capitalizing on the versatile properties of ethylene glycol (EG) as both a solvent and a reducing agent. Hydrazine is employed as a co-reducing agent to enhance the synthesis process further. Our methodology uses the polyol-mediated approach to prepare Ni and Fe-based sulfides/selenides derived from noncritical raw materials. This innovative technique holds the potential to yield catalysts that are not only highly efficient but also sustainable, making substantial contributions to the progression of hydrogen production methods. By fostering greener and economically viable practices, these catalysts play a pivotal role in driving forward environmentally friendly hydrogen production technologies.

RESULTS AND DISCUSSION

Morphological Characterization: Scanning and transmission electron microscopy (SEM, TEM) characterized the synthesized nanostructured catalysts, showing the nanostructured clusters' assembly.

Electrochemical Performance: NiFeS_x/NiFeSe_x catalysts were evaluated using a three-electrode setup in a 0.1 M KOH electrolyte and 1 M KOH. The 40% Fe content-containing NiFeSex catalyst exhibited superior performance. The FeNiS_x showed a promising industrial-relevant current density of 1A/cm² at a low voltage of 1.8V, and the material was tested in the real device later with 1 M KOH electrolyte.

CONCLUSIONS

- Study focus: Saline or low-grade water electrolysis for greener hydrogen production.
- Methodology: Polyol-mediated synthesis utilized to develop NiFeSeX electrocatalysts.
- Catalyst efficiency: Demonstrated promising performance.
- Sustainability: Highlighted potential for eco-friendly hydrogen production.
- Industrial scalability: Offers further promise for large-scale applications.




Figure 1: Single cell testing (a) FeNiS_x b) FeNiSe_x in Single cell electrolyser at different tempertaures.

Acknowledgements

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Abstract

Exploring the energy-saving potential of wastewater treatment plants under optimized discharge limit regulation			
Najafi, N. ¹ , Ryan, P. C ³ , Doherty, E. ^{1,2} , Clifford, E. ^{1,2}			
1. Civil Engineering, School of Engineering, University of Galway			
2. Ryan Institute, University of Galway			
3. Civil, Structural and Environmental Engineering, School of Engineering, University College Cork			
INTRODUCTION			
In recent decades, rising energy costs and stringent environmental regulations have heightened concerns about energy consumption within the water sector ¹ . Among various water sectors, the energy-intensive nature of wastewater treatment plants (WWTPs) poses a global challenge ² , consuming approximately 25% of the world's water sector electricity and accounting for around 3% of global greenhouse gas emission ³ . Aeration, sludge			

settling with pumping, and solids dewatering are major energy consumers in these processes⁴. However, WWTPs also offer significant energy-saving potential, highlighting the importance of reducing energy demand in wastewater sector and minimizing environmental footprint⁵.

MATERIALS AND METHODS

The effects of various WWTP characteristics (e.g. plant size, loading rates, technologies applied) on energy consumption are well researched, however, little attention is given to the possible negative effects of stringent discharge regulations (which often require more energy-intensive processes) on energy consumption. Discharge regulations are typically calculated to provide effective receiving waters protection in worst-case scenario (e.g. low assimilative capacity). However, if it were possible to vary the discharge regulations seasonally, taking into account varying assimilative capacity, then there may be an opportunity to enable WWTPs to sufficiently protect the receiving water whilst also minimising the energy requirement.

RESULTS AND DISCUSSION

To address this gap in knowledge, this study proposes investigating the relationship between discharge regulations and energy consumption of WWTPs. Furthermore, this work will also analyse how changes to discharge limits or seasonal variation in discharge limits could impact energy consumption and resulting greenhouse gas emission. The next phase of this research will involve analysing available Irish data on WWTP energy consumption to assess the impact of variable regulations on energy usage under different scenarios. The final stage of research aims to evaluate the trade-offs between energy consumption and enhanced discharge limits using life cycle assessment (LCA) methodologies.

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Abstract

Bio-synergistic Valorisation of residual forage biomass: Butyric acid and biogas production	
POOJA ₁ , Nzeteu.Corine ₁ , McAuliffee.Olivia ₂ , O'Flaherty.Vincent ₁ .	
1. School of Biological and Chemical Sciences, Microbial Ecology Lab and Ryan Institute	
2. Teagasc Food Research Centre, Moorepark, Co. Cork, Ireland	

The European Union (EU) faces a serious challenge in redefining its protein supply chain to ensure food security and environmental sustainability. There is an increasing interest in exploration of sustainable biomass options for protein production, and, the green bio-refinery concept holds significant potential to co-produce technical products and bioenergy alongside food and feed. While the prospect of extracting protein from grass looks promising, the financial success of this venture hinges on maximising the valorisation efficiency of the entire grass crop-turning every blade into a valuable resource. This study explored the potential of converting the residual press cake fraction after wet fractionation to maximum value, post-protein extraction, in grass bio-refineries. Intact Lolium perenne and its press cake fractions were investigated for biogas and valuable by-product (butyric acid) production. Biochemical Methane Potential assay indicated similar methane yields from intact and fractionated L. perenne of 222±17.28 and 242±10.28 ml g⁻¹ volatile solids (VS), respectively. During fermentation, the butyric acid yield was in the same range for the intact *L. perenne* and its press cake at 2.54 and 2.85g COD L⁻¹, respectively. This study suggests that an appealing strategy could be the optimization of the press cake fraction for high-value products, volatile fatty acids, particularly butyric acid along with subsequent biogas generation. The insights provided in this study will open up new processes and are pivotal for transitioning from linear to circular and bio-based economy.



Abstract

Dietary supplementation with rapeseed oil and cake on animal performance, methane emissions, and digestibility of beef cattle

NT Folliard ^{1,2}, Emily Roskam^{1,2}, V O'Flaherty², SM Waters², DA Kenny¹

¹ Teagasc, Animal and Bioscience Research Department, Animal and Grassland Research and Innovation Centre, Teagasc, Grange, Dunsany, Meath, Ireland
²UoG, School of Biological and Chemical Sciences, University of Galway, University road, Galway, Ireland

Ireland is legally bound to decrease agricultural GHG emissions by 25% by 2030. Anti-methanogenic feed supplements, particularly those from natural sources or by-products, could play a key enabling role. Oilseed rape (Brassica napus L) produces fatty acid-rich by-products that could potentially reduce rumen methanogenesis and positively affect meat intramuscular fat. Cold pressed rapeseed cake byproduct use would improve ration ingredient circularity. Our objective was to examine fatty acid supplementation from rapeseed ingredients on dry matter intake (DMI), average daily gain (ADG), gaseous emissions, haematology and poly unsaturated fatty acid (PUFA) content of the longissimus dorsi muscle of beef cattle fed a finishing diet. Fifty four crossbred Charolais steers and heifers (384 kg) were offered concentrates at 41% of total DMI containing either an unsupplemented control (CON), rapeseed cake (RSC) or rapeseed oil (RSO). Rapeseed oil and cake dietary inclusion (2.5 and 14.5%, respectively) was balanced on oil, total fatty acid, PUFA and mono unsaturated fatty acid content. Diets were offered with ad libitum grass silage. Feed intake and gaseous emissions were recorded over 88 days. Cattle were weighed weekly. Ultrasonic muscle and fat deposition was recorded on days 1 and 87. Blood samples were collected on days 10, 53, and 88. Biopsies of the longissimus dorsi muscle were collected on day 89. Treatment had no effect on DMI however, RSC reduced ADG (P < 0.05). RSC and RSO decreased enteric CH₄ by 8% compared to CON (P < 0.05). Production of rumen CO₂ was similar although RSO reduced H₂. Serum HDL and LDL cholesterol concentrations increased for RSC and RSO (P < 0.05). Diets did not affect muscle and fat accretion or muscle fatty acid composition (P > 0.05). Findings suggest RSO has potential for anti-methanogenic supplementation, reducing emissions without affecting animal performance, with consistent efficacy and no regulatory barriers.

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Abstract

Climate change effect on rain erosion rate in wind turbines in Ireland using CMIP6 GCMs Farzaneh Azarkaman¹, Jamie Goggins^{1,2}, William Finnegan^{1,2}

- 1. SFI MaREI Centre for Energy, Climate and Marine, Ryan Institute & School of Engineering, University of Galway, H91 TK33 Galway, Ireland.
- 2. Construct Innovate, University of Galway, H91 TK33 Galway, Ireland;

Climate change has a significant effect on future life and energy production is not an exception. Developers and decision-makers need to have a thorough understanding of how climate change affects erosion rates, especially at the leading edge of turbine blades, given the growing use of wind turbines and the ever-expanding plans for their future deployment. A common problem that limits the wind turbines' annual energy production capacity is leading edge erosion caused by raindrop impact, leading to a significant loss in the aerodynamic performance of the wind turbine blades. Erosion rate is intimately related to meteorological data and rainfall patterns, both of which are subject to alteration due to climate change.

In this study, five different pathways (SSP1-2.6, SSP2-4.5, SSP3-7.0, SSP4-6.0) of three Global Climate Models (GCM) from Coupled Model Intercomparison Project phase 6 (CMIP6) are used for precipitation with three-hour frequency in Ireland. These GCMs' data are bias-corrected with the method of empirical quantile mapping and the multi-model ensemble mean of bias-corrected data is evaluated. The historical period is considered from 1950 to 2015, and the future data from 2016-2099. Rain erosion has a direct relationship to the intensity of rain by considering the Springer method. So, the result of this analysis can be used as a tool to compare the erosion rate in future to the current rate. This endeavour serves not only as a pertinent case study but also as an essential contribution to the broader understanding of how climate change affects critical components of renewable energy infrastructure.

INTRODUCTION

Climate change could have a huge impact on future climate as well as industries such as power generation. Wind energy, not only on generating power would be affected but also can be effect on maintenance. Leading Edge Erosion is phenomena that have huge impact on wind turbine performance. It is crucial to estimate the effect of climate effect on the rate of the erosion. In this study the region of interest is Ireland island.

MATERIALS AND METHODS

This study considered 5 future scenarios, SSP1-2.6, SSP2-4.5, SSP3-7.0, SSP4-6.0 and SSP5-8.5 predictions, while SSP1-2.6 and SSP5-8.5 are the lowest and highest emissions scenario. Climate models exhibit systematic errors in their absolute outputs, such as temperature or precipitation estimates. For reduce the effect of these errors' bias correction would apply on the data. The assumption here is that the same error that happened in historical modelling is on future data. In this work Empirical Quantile Mapping (EQM) applied on GCM historical data to map it on observed data.

RESULTS AND DISCUSSION

This study shows how the perception change across the Ireland from 2015 to 2100. The results also studied in Galway wind park which is the biggest wind park in Ireland. The results show that in this location, especially in SSP5-8.5 and SSp4-6.0 the heavy rain increases in all models which means higher rate of erosion in future may happen in wind turbines.



Abstract

Supplementation with a calcium peroxide additive mitigates enteric methane emissions in beef cattle
Roskam, E ₁₂ , Kenny, D. A ₁₃ , O'Flaherty, V ₂ , Kelly, A. K ₃ , Waters, S. M ₂
 Animal and Bioscience Research Department, Teagasc Grange, Meath, Ireland School of Biological and Chemical Sciences, University of Galway, Ireland UCD school of Agricultural and Food Science, University College Dublin, Ireland

In Ireland, the agricultural sector is responsible for 38% of GHGs, 60% of which are methane (CH₄). Globally, GHGs need to be reduced to adhere to legally binding targets. While research into dietary supplementation with anti-methanogenic feed additives has proliferated, there are still limited products showing consistent CH₄ reductions, many of which cannot be pelleted due to sensitivity to temperature and pressure. Calcium peroxide (CaO₂) is a widely available, non-toxic, inexpensive compound, which has been shown to have anti-methanogenic properties based on modulating the oxidation-reduction potential of the rumen.

In this study, the effect of twice daily supplementation of CaO_2 to beef bulls on CH_4 and H_2 emissions and animal productivity was assessed. Seventy two beef bulls offered a 60:40 forage:concentrate diet were allocated silage each morning (0900h) and concentrates at 0800h and 1500h. Following a 7d covariate period, animals were offered 1 of 4 treatments; Control (unsupplemented), Low (1.35% CaO₂), High (2.25% CaO₂) and Pellet (High, pelleted) (n=18). All concentrates were formulated in a coarse ration, except for Pellet. CH_4 and H_2 were measured using GreenFeed systems. Data were analysed using ProcMixed, SAS 9.4.

No effect on animal ADG or FCR was observed (P>0.1), however High reduced DMI compared to Control (P<0.05). All treatments reduced CH₄ emissions when expressed per day, per kg ADG and per kg DMI (P<.0001). Low reduced CH₄ parameters by 17-22%. High and Pellet reduced CH₄g/d, g/kg ADG and g/kg DMI by 28 and 27, 33 and 24, and 20 and 27% (P<.0001) respectively. A 36, 35 and 32% reduction in H₂ (P<.0001) was observed for Low, High and Pellet. CaO₂ can successfully endure the pelleting process and reduce CH₄ and H₂ emissions with no negative effects on animal production, making it a viable CH₄ mitigation option for pasture based systems with concentrate supplementation.



Abstract

Analysis of connections in a multi-storey modular CLT building using Irish timber

Kashyap, R.1, O'Ceallaigh, C.2, McGetrick, P.J.1, Harte, A.M.1

1. Timber Engineering Research Group, Ryan Institute, University of Galway

2. Department of Building and Civil Engineering, Atlantic Technological University

INTRODUCTION

Cross-laminated timber (CLT) has emerged as an excellent material in terms of structural properties and environmental impact due to the shift in focus towards sustainable construction materials. Ireland has an increasing supply of Sitka spruce timber primarily graded as C16. The primary structural timber grade used for the manufacture of CLT across Europe is C24-grade, so most research data is only available for C24-grade CLT. Commonly available connectors for connections in multi-storey modular buildings constructed using C16-grade CLT. Angle brackets are typically used for wall-to-floor or wall-to-ceiling connections and steel plates are mainly used for module-to-module connections. Connections have been tested under shear and compression loads to determine their behaviour for CLT panels manufactured using C16-grade Irish timber to achieve an optimal connection design. In parallel, a finite element model of these connections is created using ABAQUS, which is validated using the experimental results.

MATERIALS AND METHODS

CLT panels are engineered wood products manufactured from at least three layers of boards glued together with adjacent layers orientated at right angles to each other and bonded together with adhesives under pressure in accordance with EN 16351. Connections using industry-standard angle brackets and plates have been examined. Rothoblaas TTF200 angle brackets fastened using three different screw lengths Rothoblaas LBS550, LBS560 and LBS570 have been tested under shear and compression loads. Rothoblaas TTP200 plates, fastened using LBS540 screws have been tested under shear loads. Numerical models for the same have been modeled using ABAQUS.



Figure 1: Specimens after compression test using TTP200 angle brackets and 3 screw lengths **RESULTS AND DISCUSSION**

The load-displacement curves from the experimental results are analysed and have provided significant information on the structural performance of these connections. They are then compared to the load-displacement curves obtained from the numerical models. Future research needs for using these connections for a modular building made of C16-grade CLT shall be identified and highlighted.



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CURIOSITY & DISCOVERY

DECISIVE DATA





Abstract

 Performances analysis of various atmospheric correction algorithms for monitoring Irish Transitional and Coastal (TrC) waterbodies using Sentinel-3 OLCI imagery

 Sajib, A.M.1234, Digatna, Mir T.M. 1234, Uddin, Md.G. 1234, Olbert, A.I. 1234

 1 School of Engineering, College of Science and Engineering, University of Galway, Ireland. 2 Ryan Institute, University of Galway, Ireland. 3 MaREI Research Centre, University of Galway, Ireland

 4 Eco-HydroInformatics Research Group (EHIRG), Civil Engineering, University of Galway, Ireland

The availability of free and open data policies has led to the wide use of remote sensing (RS) products for assessing water quality (WQ) in the world. According to the literature, multispectral satellite products, including Landsat 8/9 OLI, Sentinel-2 MSI, Sentinel-3 OLCI, etc. RS products most widely utilize in the field of water quality monitoring. Among them, European Space Agency (ESA) recommended Sentinel-3 OLCI (Ocean and land color instrument) for conducting wide-scale observations of the optical and in-optical properties of ocean waters. Several recent studies have identified various challenges, including atmospheric conditions, surface reflection, adjacency effects, and sensor characteristics in RS products. For the purposes of the reliable and accurate assessment of WQ (various indicators like dissolved oxygen (DOX), pH, chlorophyll a (CHL) etc.), it is essential to eliminate the effect of the atmosphere from the RS products. However, the research aim was to compare the performance four widely used atmospheric correction (AC) algorithms such as C2RCC, ACOLITE, L2gen, POLYMER etc., using Sentinel-3 OLCI data in order to retrieve the dissolved oxygen (inactive), and chlorophyll a (active) in Irish TrC waterbodies. To assess the performance of AC, the study has developed 8188 models using the 25 ML/AI algorithms. The performance of the algorithms were evaluated using five identical metric R², RMSE, MSE, MAE, PABE. Based on the initial assessment, the ACOLITE-AC could be effective to obtain more accurate WQ assessment, particularly DOX, and CHL using the extreme gradient boosting algorithm. The result of the research could be helpful for optimizing the atmospheric intervention in RS process in order to obtain accurate assessment of WQ in TrC waterbodies, Ireland.

Keywords: Atmospheric correction, Sentinel-3 OLCI, Water quality, Remote sensing, Machine learning, Irish waters



Abstract

Enhancing Translation Quality by Leveraging Semantic Diversity in Multimodal Machine Translation Hatami, Ali₁, Buitelaar, Paul₁, Arcan, Mihael₂.

Insight SFI Research Centre for Data Analytics, Data Science Institute, University of Galway, Ireland
 Lua Health, Business Innovation Centre, University of Galway, Ireland

INTRODUCTION

Despite improvements in neural machine translation models to capture the entire textual context, word sense disambiguation remains challenging. Multimodal Machine Translation (MMT) integrates visual information to enhance text-only translation models. However, the effectiveness of using visual information on translation quality varies based on the text being translated. The study aims to identify sentences where visual content improves MMT. We utilise Latent Semantic Analysis (LSA) and Sentence-BERT (S-BERT) to calculate ambiguity scores at the sentence level. Our approach enhances translation quality for English-German on the Multi30k dataset in terms of the BLEU metric.

METHODOLOGY

We employed semantic diversity to quantify lexical ambiguity for nouns and applied these scores to compute ambiguity at the sentence level. Our study explored various thresholds of sentence ambiguity to optimise BLEU scores in the evaluation dataset, selecting translations from text-only and Multimodal. We assessed textual similarity using LSA and S-BERT which closer vectors indicated higher cosine similarity and lower ambiguity scores. At the sentence level, we computed ambiguity scores using arithmetic and geometric mean functions. By assigning semantic diversity thresholds to these scores, we determined whether to utilise text-only or Multimodal translation for a given sentence.

RESULTS AND DISCUSSION

In Figure 1, the results of BLEU scores for LSA and S-BERT are presented in Mean and G-Mean. The overall BLEU scores for the text-only model (blue dashed line) and multimodal model (red dashed line) are 37.92 and 39.45, respectively. Unlike S-BERT, LSA approaches exhibit higher BLEU scores at certain sentence ambiguity thresholds compared to the baseline multimodal model. Specifically, LSA's approach based on G-Mean demonstrates an improvement over the multimodal baseline model for sentence ambiguity scores less than 1.58, after which G-Mean drops below the quality of Mean.





Abstract

Performance analysis of machine learning/artificial intelligence models for trend prediction of various hydro-climatic variables		
<u>Bamal, A.</u> ^{1, 2, 3, 4} , Uddin, M.G. ^{1, 2, 3, 4} , Olbert, A. I. ^{1,2,3,4}		
 School of Engineering, University of Galway, Ireland Ryan Institute, University of Galway, Ireland MaREI Research Centre, University of Galway, Ireland Eco-HydroInformatics Research Group (EHIRG), Civil Engineering, National University of Ireland Galway, Ireland 		
Trend analysis is a relevant aspect of assessing the changes in hydro-climatic variables over time to understand the climate change progression in any region along with its impacts on other domains such as water quality, ecological status, socio-economic growth, etc. In the current scenario, a range of tools and techniques are widely used for trend analysis such as advanced statistical approaches, machine learning/artificial intelligence (ML/AI) techniques, etc. This study aims to identify the best ML/AI model to predict the trends of eight hydro-climatic variables including temperature, precipitation, evaporation, windspeed, surface runoff, total runoff, solar radiation, and relative humidity in the context of Ireland. The study utilized 15 ML/AI algorithms to identify the best model using evaluation metrics including the calculation of R ² (correlation coefficient), root mean square error (RMSE), mean square error (MSE) and mean absolute error (MAE). Amongst the eight variables, the variables with best performance in terms of evaluation metrics were selected for final presentation in this study.		
Based on the performance of 15 ML/AI algorithms, two hybrid models: (i) CNN+RNN+DNN (Convolutional Neural Network (CNN) + Recurrent Neural Networks (RNN) + Deep Neural Network (DNN)); and (ii) ANN-MLP (Artificial Neural Networks- Multilayer Perceptron) outperformed other models in terms of performance metrics during both training and testing phases. Amongst the studied hydro-climatic variables, the hybrid model ii (ANN-MLP) implied the best performance for solar radiation (training: R ² = 0.96, RMSE= 0.03, MSE= 0.00, MAE= 0.04; testing: R ² = 0.97, RMSE= 0.04, MSE= 0.00, MAE=0.03) while the hybrid model (i) (CNN+RNN+DNN) outperformed for evaporation (training: R ² = 0.74, RMSE= 0.48, MSE= 0.23, MAE= 0.34; testing: R ² = 0.79, RMSE= 0.08, MSE= 0.00, MAE= 0.03).		
The results of the study imply that the hybrid models can be successfully used for prediction of trends and outperform the standalone ML/AI models. Hence, there is a potential for world-wide applications of the proposed modelling approach, however, the proposed solution requires further validation for various hydro-climatic data and testing the model sensitivity for various domains and their spatio- temporal resolutions.		



Abstract

MultiOmicsIntegrator – MOI: An integrated solution for omics analyses	
Bianca A. Pasat ^{1,2,3,4} *, Eleftherios Pilalis ³ , Katarzyna Mnich ^{1,5} , Afshin Samali ^{1,5} , Aristotelis	
Chatziioannou ^{2,3} , Adrienne M. Gorman ^{1,5}	
¹ Apoptosis Research Centre, School of Biological and Chemical Sciences, University of Galway,	
Ireland	
² Center of Systems Biology, Biomedical Research Foundation of the Academy of Athens, 4 Soranou	
Ephessiou str, 11527, Athens, Greece	
³ e-NIOS Applications PC, 196 Al Syggrou Ave. 17671, Kallithea, Greece	
⁴ Science Foundation Ireland, CRT, Genomics Data Science, University of Galway, Ireland	
⁵ CÚRAM, SFI Research Centre for Medical Devices, University of Galway, Ireland	
* Corresponding author	

RNA sequencing is revolutionizing transcriptomic analysis through the unbiased monitoring of genomic expression and regulation with the aid of powerful biotechnologies coupled with powerful analytical techniques. In particular, analysis of gene and isoform expression levels is becoming critical for the detailed understanding biochemical mechanisms. In addition, integrating RNA-seq data with other omics data types, such as proteomics and metabolomics, provides a strong approach for consolidating our understanding of biological processes across various organizational tiers and thus promoting the identification of potential therapeutic targets. Integration of multi omics also serves as a valuable asset in advancing personalized medicine initiatives.

We present our nextflow pipeline, called MultiOmicsIntegrator (MOI), an inclusive pipeline for comprehensive omics analyses. MOI represents a unified approach that performs in-depth individual analyses of diverse omics, including mRNAs, proteins, lipids, and miRNAs, providing a holistic view of biological systems. In addition, one of its key features is the ability to address isoform-level analysis of mRNA, providing various tools to facilitate the comprehensive understanding of gene regulation processes. In addition, tools for functional annotation and secondary structure prediction of RNA molecules further promote the effort to unravel the complex networks where these molecules reside. Finally, MOI has tools to integrate simultaneously multiple and diverse omics datasets, fostering a deeper understanding of intricate biological interactions. MOI offers a modular approach that performs specific tasks. Modules can be combined to form a complete pipeline, making it flexible and adaptable to differences in analysis requirements. We demonstrate the utility of MOI through two scenarios: one focusing on isoform analysis in patients with Parkinson's Disease, and the other involving multi-omics integration across a broad spectrum of cancer cell lines sourced from CCLE.

Availability of code:

https://github.com/ASAGlab/MOI--An-integrated-solution-for-omics-analyses



Abstract

Multiscale instability analysis of layered magnetoactive elastomers

Chen Xie ^a, Andrei V. Cherkasov ^a, Quan Zhang ^a, Parag Pathak ^b, Stephan Rudykh ^{a,b,} ^a School of Mathematical and Statistical Sciences, University of Galway, Galway H91 TK33, Ireland ^b Department of Mechanical Engineering, University of Wisconsin – Madison, Madison, WI 53706, United States

Magnetoactive elastomers (MAEs) are composite materials whose mechanical behavior can be tuned by an external magnetic field. This characteristic leads to numerous applications such as soft robots, sensors, and noise barriers. This work aims to provide a guideline to actively and remotely control microstructure transformations and mechanical properties in magnetoactive soft composites by triggering magnetic-induced instabilities. For this purpose, a framework to perform instability analysis of MAEs is proposed. Specifically, take the laminates as an example, numerical and analytical models of layered MAEs with soft/hard magnetic inclusions are developed based on the finite element method and classical magneto-elasticity theory. Buckling and post-buckling analysis are performed to predict the onsets of instabilities at the microscopic and macroscopic length scales. Based on the established models, we obtained the relationships between critical stretch (critical wavelength) and magnetic field level. Further, we have studied the effect of volume fraction, additional invariants, and initial susceptibility on the onset of magneto-mechanical instabilities.



Abstract
Stimulation of Mechanosensitive Ion Channels to affect Macrophage Polarization and the
Cargo of their EVs
Whelan, C. ^{1,2,3} , Monaghan, M. G. ⁴ , El-Haj, A. J. ⁵ , Brennan, M. ^{1,2,3}
¹ Regenerative Medicine Institute (REMEDI), School of Medicine, University of Galway
² Curam, SFI Research Centre for Medical Devices, University of Galway
³ Biomedical Engineering, College of Science and Engineering, University of Galway
⁴ Trinity College Dublin
⁵ University of Birmingham

INTRODUCTION

It is widely accepted that cytokines such as IFN- γ /LPS and IL-4/IL-13 can polarise macrophages to the pro-inflammatory (M1) and pro-wound healing (M2) phenotypes, respectively. However, these methods of macrophage polarisation only yield 10-20% of the desired population and certain cytokines can increase apoptosis further reducing this yield (1, 2). Recently, mechanostimulation has been also proven to modulate cell phenotypes (3, 4). However, there are conflicting opinions among researchers regarding how mechanostimulation affects macrophage polarisation (5, 6). The aim of my project is to specifically activate mechanosensitive ion channels on macrophages and determine how this affects their phenotype and the cargo of their extracellular vesicles (EVs).

MATERIALS AND METHODS

Initially macrophages derived from THP-1s and human blood monocytes will be polarised with cytokines, and a panel of M1 and M2 markers will be selected using ELISAs, flow cytometry and RT-PCR. Then remotely controlled magnetic nanoparticles tagged with antibodies against the mechanosensitive ion channels Piezo1 and TREK1 will be used, alongside cytokines, to determine how the activation of these ion channels effects macrophage polarization. Following mechanical stimulation, polarisation will be verified using two-photon fluorescence lifetime imaging, ELISAs, flow cytometry and RT-PCR. EVs will be isolated by size exclusion chromatography and they will be characterised by nanoparticle tracking analysis, BCA assays, transmission electron microscopy and flow cytometry.

DISCUSSION

We expect that this research will better emulate the native environment macrophages experience *in vivo* by utilising both chemical and mechanical stimuli compared to chemical stimuli alone. We hypothesize that this combination will affect macrophage polarization and their EV cargo.

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Abstract

FOXP1 Dysregulation and its Association with Neuropsychiatric Disorders and Cognitive Function		
<u>Ali, Deema1</u> , Morris, Derek1		
1. Centre for Neuroimaging, Cognition and Genomics, School of Biological and Chemical		
Sciences, University of Galway, Galway, Ireland.		

INTRODUCTION

Rare mutations in *FOXP1* (Forkhead-box protein P1), a transcription factor crucial for cortical neural development, cause FOXP1 syndrome, which is characterized by developmental delays, intellectual disability, with or without autistic features. Common SNPs within the gene are associated with schizophrenia (SCZ) and cognitive function. In this study, we investigated FOXP1's contribution to these phenotypes using RNA-seq data from FOXP1 knockout animal models. These data were available from cortical neural stem cells from embryonic mice and cortical tissues across different postnatal developmental stages (P0, P7, P47).

MATERIALS AND METHODS

Pairwise comparisons and time-course expression analysis were conducted on the RNA-seq data from the different developmental stages. Linkage disequilibrium score regression was performed to investigate if differentially expressed genes (termed gene-sets) were enriched for heritability contributing to the SCZ and cognitive function. Cell type enrichment analysis was conducted to identify the individual affected cell types and brain regions. Gene ontology analysis was performed to elucidate the underlying biological mechanisms impacted by FOXP1 knockout.

RESULTS AND DISCUSSION

Across all stages, FOXP1 gene-sets showed enrichment for SNP-based heritability related to educational attainment (EA) and/or intelligence. Nearly all FOXP1 gene-sets were enriched for SCZ heritability, with the highest enrichment observed at the P47 stage. FOXP1 gene-sets from both P7 and P47 stages exhibit significant enrichment in excitatory glutamatergic neurons within both the frontal and posterior cortex. FOXP1 is involved in neurogenesis and synaptic signalling functions across all developmental stages. In the later stages (P7 and P47), FOXP1 is particularly associated with the regulation of ion transport and the G protein-coupled receptor signalling. Time-course expression analysis identified 1,128 significant genes across developmental stages, enriched for SCZ and EA heritability, and involved in similar biological processes. Overall, FOXP1 disruption across stages dysregulates genes associated with SCZ risk and cognitive function, suggesting a diverse range of biological pathways involved in their aetiology.



Abstract

Flare Star: EQ Pegasi
Ní Chonchubhair D. ¹
¹ School of Mathematical and Statistical Sciences

Flaring is common in magnetically active stars and can be observed across the electro-magnetic spectrum, with the Sun being no exception. The most interesting solar flares are those extreme events that also produce coronal mass ejections (CME) that can result in potentially debilitating space weather events here on Earth. Hundreds of 'habitable zone' exoplanets have been to date, discovered around nearby stars, many of which are more active than our Sun - could these planets survive long term exposure to more powerful CMEs? EQ Peg is a nearby red dwarf flare star binary system with a period of ~ 180 years. We present results of a 6 hour observation of the EQ Peg system with the I:IO photometer on the Liverpool Telescope. Both components, EQ Peg A and EQ Peg B, were found to produce flares. EQ Peg A was found to be particularly active with a complex pattern of flare events occurring towards the end of the optical observations. We speculate on the likely association of this flare event with a CME, particularly in light of the recently discovered 2.3 Jupiter mass size planet orbiting EQ Peg A.



Abstract

The challenges of using machine learning models in psychiatric research and clinical practice		
Ostojic, D. ₁ , Lalousis, P. A. _{2,3} , Donohoe, G. ₁ , Morris, D. W. ₁ *		
¹ School of Biological and Chemical Sciences and School of Psychology, Centre for Neuroimaging, Cognition and Genomics (NICOG), University of Galway, Ireland.		
² Department of Psychosis Studies, Institute of Psychiatry, Psychology & Neuroscience, King's College London, London, United Kingdom.		
₃ Section for Precision Psychiatry, Department of Psychiatry and Psychotherapy, Ludwig-Maximilian- University Munich, Munich, Germany.		
The complex nature of heterogeneous psychiatric disorders means that scientists and clinicians employ a wide range of clinical, endophenotypic, neuroimaging, genomic, and environmental data to uncover knowledge about the biological basis of psychiatric illness before attempting to translate		
to uncover knowledge about the biological basis of psychiatric illness before attempting to translate that knowledge into improved clinical care. Machine learning (ML) is an automated process that extracts patterns from data and can supersede conventional statistical methods by detecting linear and non-linear relationships in large multidimensional datasets. This offers the opportunity to		
enhance our understanding of psychiatric disorders using multi-modal data, leading to improved diagnosis, prognosis and treatment. ML models are often employed to solve problems such as classification, regression, dimensionality reduction or clustering using multi-modal data. The current review provides an in-depth examination of and offers practical guidance for the challenges		
review provides an in-depth examination of, and offers practical guidance for, the challenges encountered in the application of ML models in psychiatric research and clinical practice. These challenges include the curse of dimensionality, data quality, the 'black box' problem,		
hyperparameter tuning, external validation, class imbalance, data representativeness, data drift and model selection. These challenges are particularly critical in the context of psychiatry as it is expected that researchers will encounter them during the stages of ML model development and		
deployment. We detail practical solutions and best practices to effectively mitigate the outlined challenges. These recommendations have the potential to improve reliability and interpretability of		
ML models in psychiatry.		



Abstract

Dynamic Malware Classification and API Categorisation of Windows PE Files using Machine	
Learning	
Syeda, D. Z. $_1$ and Dr. Asghar . M. N. $_1$	
1. School of Computer Science, University of Galway, Galway, Ireland.	

The rise of malware attacks presents a significant cyber security challenge, with advanced techniques and offline command-and-control (C2) servers causing disruptions and financial losses. This paper proposes a methodology for dynamic malware analysis and classification using a malware Portable Executable (PE) file from the "Malwarebazar" repository. This paper proposed effective strategies to mitigate the impact of evolving malware threats. For this purpose, a five-level approach for data management and experiments is utilised: (1) Generation of the customised dataset by analysing a total of 582 malware and 438 goodware samples of Windows PE files; (2) Feature extraction and feature Scoring based on Chi2, and Gini importance; (3) Empirical evaluation of six state-of-the-art baseline machine learning (ML) models including Logistic Regression (LR), Support Vector Machine (SVM), Naive Bayes (NB), Random Forest (RF), XGBoost (XGB), and k-Nearest Neighbour (KNN) on the curated dataset; (4) Malware family classification using VirusTotal APIs; and (5) finally, categorised 23 distinct APIs from 266 Malware APIs. According to the results, Gini's method takes a holistic view of feature scoring, considering a wider range of API activities. The RF achieved the highest Precision of 0.99, Accuracy of 0.96, Area Under Curve (AUC) of 0.98, and F1-score of 0.96 with 0.93 true positive rate (TPR) and 0.0098 false positive rate (FPR) among all applied ML models. The results show that Trojan (27%) and Ransomware (22%) are the riskiest among 11 malware families. Windows-based APIs (22%), File system (12%) and Registry manipulation (8.2%) showcase their importance in detecting malicious activity in API categorisation. This paper considers a dual approach for feature reduction and scoring, resulting in an improved F1-score (2%) and the inclusion of AUC and Specificity metrics distinguishes it from existing research (section (5)). The newly generated dataset is publicly available in the GitHub repository (section (8)) to facilitate aspirant researchers for dynamic malware analysis.

Keywords: Malware; Dynamic Malware Analysis; Feature Extraction; Feature Scoring; Malware Classification; API Categorisation; Dataset Generation; ML Models



Abstract

First in vitro comparison of time-dependant DNA damage response in short-lived and long-lived bat fibroblasts to ionizing radiation exposure and comparison to model organisms.

Skujina, I. 1

1. School of Biological and Chemical Sciences, University of Galway

Although ageing is a complex and multifaceted process leading to widespread functional decline and age-associated illnesses, increasing evidence points to the DNA damage and consequent genome instability that is affecting most, if not all, aspects of the ageing process. DNA is constantly being damage by both internal and external agents. However, some species have evolved more efficient DNA damage responses (DDR) protective of both cancer and ageing. Understanding ageing-related molecular pathways in long-lived animals is challenging, with most breakthroughs obtained using inbred and short-lived laboratory model organisms, which are poor models for long-lived and outbred species such as humans. Bats are a highly diverse group of mammals that despite the extra metabolic load caused by flight can far exceed the maximum longevity of other similar-sized mammals and as such offer an excellent model to discover new molecular insights and solutions to slow down the ageing process.

We hypothesise that long-lived bats (e.g. *Myotis myotis*) will have more effective DDRs throughout their lifespans than more short-lived species with similar life-histories (e.g. *Molossus molossus*). *In vitro* measurements of DDR effectiveness in cultured bat primary fibroblast cells in comparison with the DDR of human and mouse cells will be used to test this hypothesis. We anticipate identifying more robust DDR in long-lived bats. We further hypothesise that cells isolated from long-lived bats will maintain more error-free mechanisms of DNA repair as they age relative to shorter lived bat species. We aim to elucidate why species of similar size and lifestyles can have widely different longevities. Our proposed work may also result in development of more biomedically relevant models of the ageing process.



Abstract

Evolution of acid resistance in a clinical isolate of Listeria monocytogenes reveals selection for altered SigB activity.			
Jialun Wu, Brenda Chanza, Ashley Reade, Conor O'Byrne.			
Bacterial Stress Response Group, Microbiology, School of Biological & Chemical Sciences, University of Galway, Galway H91 TK33, Ireland.			
Listeria monocytogenes is a food-borne pathogen that causes life-threatening disease when it infects immune-compromised individuals. We have previously isolated a clonal complex 1 (CC1) <i>L. monocytogenes</i> strain, MQ140025 from a patient in Ireland. This strain carries mutations in the <i>sigB</i> operon (RsbU Q317*, RsbX N77K), which encodes SigB and its regulators. In <i>L. monocytogenes</i> , SigB mediates general stress response and promotes host entry. This strain exhibits reduced SigB activities and compromised acid resistance. While we have previously shown that loss-of-functions <i>sigB</i> operon mutations are prevalent among wild isolates and they confer selective advantages under mildly stressful conditions, it is intriguing to observe them in a clinical isolate as SigB activity is important for surviving stomach transit and intestinal epithelial cells entry. We hypothesize that the SigB activities can easily loose and regain in <i>L. monocytogenes</i> to favour the survival or growth of this bacterium when selective pressure occurs. To test this, the cultures of strain MQ140025 were subjected to lethal acidic challenge and recovery cycles (Figure 1) to select for acid resistant derivatives (ARD). Acid resistance rapidly			
100 μL sample +			



Figure 1 Schematic presentation of *in vitro* evolution experimental setup, three parallelly cultures of strain MQ140025 were repeated exposed to lethal acid challenges and recovered. pH 3 was applied as lethal acid challenge for day 1, day 2, and day 3 while pH 2.5 was applied for day 3 and day 4 for time specified.

developed in all three independent evolution setups and ARDs were isolated from all three evolved cultures. ARDs displayed lower motility (suppressed by SigB) and expressed SigB-dependent genes at higher levels. Interestingly, colonies of these ARDs manifested unusual surface structure when cultivated on brain heart infusion plates supplemented with congo red, suggesting that SigB has alternative roles in the synthesis of extracellular polymeric substance (EPS) in this clinical strain. In conclusion, we observed that SigB activity can be readily regained when lethal environmental pressures occurs and that SigB may have previously unacknowledged roles in EPS production.



Abstract

A Comprehensive Experimental and Kinetic Modelling Study of Methyl Tert-Butyl Ether Combustion

Jintao, C.1

1. School of Biological and Chemical Sciences

A comprehensive understanding of the combustion chemistry of methyl tert-butyl ether (MTBE) is of key importance in its application as an additive in gasoline fuels. Ignition delay times (IDTs) of MTBE/air mixtures have been measured in both a high-pressure shock tube (HPST) and in a rapid compression machine (RCM) at equivalence ratios of 0.5, 1.0, and 2.0 in air, at pressures of 10 and 30 bar over the temperature range 600 - 1350 K. Species profiles for MTBE oxidation were obtained in a jet-stirred reactor (JSR) at 1 bar, at equivalence ratios of 0.5, 1.0, and 2.0 in the temperature range 700 - 1100 K.

A detailed reaction mechanism, composed of 816 species and 4353 reactions, has been developed and predicts well all of the experimental data obtained in this work and also the ones in the literature. A sensitivity analysis reveals that the elimination reaction of MTBE is important, and significantly inhibits fuel reactivity at temperatures above 1300 K. At intermediate temperatures (850 - 1300 K), the reaction MTBE + $\dot{O}H = T\dot{C}_4H_8OCH_3 + H_2O$ plays a crucial role in promoting the reactivity of MTBE oxidation, whereas the reaction MTBE + $\dot{O}H = TC4H9O\dot{C}H2 + H2O$ is the most inhibiting reaction. At low temperatures (600 - 850 K), the isomerization reaction of TC4OCO₂-1 = TC₄OCO₂H-2 significantly promotes the reactivity. Conversely, the 2TC₄OCO₂-1 <=> 2TC₄OCO-1 + O₂ inhibits reactivity the most. The NTC behavior in MTBE oxidation can be explained by the competition between the reaction involving the formation and consumption of cyclic ethers from TC₄H₈OCH₃ radicals and the reactions associated with the formation and consumption of carbonyl hydroperoxide species.



Abstract

Multivariate longitudinal functional data analysis with applications in biomechanics	
Andrew, J _{1.2} , Simpkin, A J _{1,2} .	
	1. University of Galway
2. SFI	Insight Centre for Data Analytics
2. 51	

INTRODUCTION

Fatigue, defined as a decline in muscular force due to exercise, affects athletes' performance and monitoring it is vital in sports. Assessing fatigue helps to optimise athletes' performance and their readiness to train. Objective assessment of fatigue is usually done in specialised laboratories that are expensive and environmentally constrained. Low-cost lightweight sensors offer a compelling alternative, but the high-throughput data they collect are complex and functional in nature. This research aims to identify and characterise the difference between fatigued and non-fatigued running and clustering athletes using wearable sensors data.

MATERIALS AND METHODS

We explored data from 19 athletes running 400M under normal/ healthy condition and again under fatigued condition with a sensor mounted on their lumbar spine. The running involved running under healthy condition followed by fatiguing protocol, and later running when fatigued. In all three segments, sensor captured six signals 256 times per second: the accelerometer in three directions (X, Y, Z) and the gyroscope in three directions (X, Y, Z). The long record of any of the six signals was broken into individual strides forming a series of functional strides arising longitudinally, combining all six signals bring a multivariate data structure. We make use of a multivariate longitudinal functional data analysis framework which utilises all the data and captures the changes throughout the run.

RESULTS AND DISCUSSION

We analysed acceleration in X, Y, and Z directions, and with our modelling framework, we demonstrate, (1) an appropriate way of summarising data from multiple signals into a better representation, (2) using these generated representations to identify and characterise fatigue throughout running, and (3) segment athletes into different groups. These findings serve as a foundation for understanding fatigue and how it differs from athlete to athlete. This will help in developing an effective personalised fatigue monitoring and assessment tool.



Abstract

Trends in Indoor Environmental Quality in Non-Domestic Energy-Efficient Buildings in Ireland:
the BENEFIT Project
<u>Fernandes, J.M.¹</u> , Byrne, M. ¹ , Collison, A. ¹ , McGrath, J. ²
1. Physics Unit, School of Natural Sciences and the Ryan Institute's Centre for Climate and
Air Pollution Studies, University of Galway, Galway, Ireland
2. Department of Physics, Maynooth University, Maynooth, County Kildare, Ireland

The 2021 Glasgow Agreement underscores the continued global emphasis on reducing carbon emissions as a key political goal, and the International Energy Agency recognizes the significance of energy efficiency advancements in their crucial role to achieve a low-carbon future. However, energy efficiency does not always equate to good indoor environmental quality (IEQ), as a consequence of compromises in ventilation rates. In recent years, a large focus of research has centred on examining the implications for energy improvements in the residential sectors. While much research has focused on energy improvements in residential settings, similar attention hasn't been given to offices and schools. Addressing indoor air quality in these environments is critical for ensuring the health, well-being, and productivity of employees and students, particularly considering the COVID-19 pandemic.

The BENEFIT project aims to conduct a comprehensive and scientifically robust assessment of the impacts of energy-efficient policies in non-domestic settings across Ireland. The study is designed to evaluate IEQ within energy-efficient office and school environments. This comprehensive approach entails capturing a diverse range of indoor settings, including different age groups of students (5 to 18 years old) and office workspaces. In this presentation, the focus is on newly constructed energy-efficient buildings in which multizone real-time monitoring and hybrid methodology is used to assess indoor environmental quality, capturing longer-term trends through precise measurements of crucial indoor pollutants (e.g., PM_{2.5}, TVOC, formaldehyde, BTEX, ozone, radon, NO₂, CO and CO₂).

Preliminary IEQ monitoring results will be presented, and these are expected to shed light on the ability of energy-efficient non-domestic buildings in Ireland to maintain a healthy indoor environment, thus addressing a significant knowledge gap. A comparative approach to assessing indoor air quality in new buildings, relative to those which have undergone an energy retrofit (which is being addressed in a separate presentation), will be considered.



Abstract

Evaluating Residential Building Performance: A Categorical Analysis of Temperature, Humidity, and CO2
<u>Memon, L.R. 1,3, Moran, P. 1,2,4</u> , Goggins, J. 1,2,3,4
1. Civil Engineering, School of Engineering, University of Galway, Ireland.
2. MaREI Centre for Marine, Climate and Energy, Ryan Institute, University of Galway,
University Road, Galway, Ireland.
3. ERBE Centre for Doctoral Training, University of Galway, University Road, Galway,
Ireland.
4. Construct Innovate, University of Galway, University Road, Galway, Ireland.
INTRODUCTION In Ireland and globally, a primary concern is whether retrofitted houses perform as promised

In Ireland and globally, a primary concern is whether retrofitted houses perform as promised to provide occupants with better indoor environment quality (IEQ), which may affect their satisfaction and health. Although there has been growing interest in the performance of retrofitted residential buildings, a post-occupancy evaluation of performance is required as evidence of improvements. This study evaluates the performance of 10 Galway homes based on indoor temperature, humidity, and CO₂ levels. All selected homes possess a Building Energy Rating (BER) of A3 or better, aligning with stringent energy-efficiency standards. These homes are scored based on the continuous monitoring of daily average temperature and relative humidity over a duration of three to twelve months to assess compliance with established comfort zones (Temperature: 18-24°C, RH: 40-60%). In addition to the scoring assigned based on meeting the comfort standards, Time of Wetness (TOW) was calculated to evaluate the risk of mould development, while CO₂ concentrations were analysed to deduce occupancy behaviour patterns and determine whether they surpass the established threshold of 1000 ppm. The collected data is graphically represented to facilitate the comparison with optimal ranges for mould growth, as well as the categorisation of potential mould colonisation.



Figure 1: Performance of one house H040

RESULTS IMPACT

The results of this study can be helpful in evaluating building performance, particularly when energy savings are contractually guaranteed. It underscores the importance of monitoring the indoor environment post-occupancy to ensure that energy efficiencies do not compromise the indoor climate. Building owners, Energy Service Companies, and local authorities will benefit from such type of assessment framework, as it will provide a concise, single-page assessment of building performance and contractual terms.



Abstract

Modelling Composition Response Data with Application to Clot Composition Observed for Acute Ischemic Stroke (AIS) Patients

Almutairi, M. 1 1. School of Mathematical and Statistical Sciences

Modelling composition response data presents challenges due to the nature of multivariate proportions for multiple elements making up the whole composition of an individual's sample. This poster investigates the modelling of composition response data, focusing on thrombotic material extracted from Acute Ischemic Stroke (AIS) patients using mechanical thrombectomy, which measures five components making up the clot composition. The aim is to model composition response considering the effects of factors that may influence changes in clot composition.

The challenges of modelling composition response data include bounded responses, continuous scale bounded between 0 and 1, correlation between multivariate responses, and multivariate responses within the sample constrained to sum to 1, as proportions of the composition of the whole sample. Using a traditional statistical analysis which assumes a normal error structure, for continuous univariate response data bounded between 0 and 1, can lead to biased and incorrect estimates. Therefore, an appropriate model like beta regression should be used for reliable parameter estimates rather than normal linear regression. Similarly, expanding to the multivariate response setting, Dirichlet regression is an appropriate modelling approach. We present results in application to the AIS patient cohort to cluster and model clot composition with candidate predictors, such as type of extraction device, hospital of procedure, etiology categorisation, and use of drug treatment tPA.



Abstract

Manufacture of Carbon Fibre Reinforced Composites Using Additively Manufactured "Lost Core" Molds
<u>Flanagan, M¹</u> . Goggins, J ¹ . Harrison, N ² . Finnegan, W ¹
 School of Engineering, Sustainable and Resilient Structures School of Engineering, Advanced Manufacturing
2. School of Engineering, Advanced Manufacturing

INTRODUCTION

"Lost core" molds are used to manufacture complex carbon fibre-reinforced composites parts. Several companies have developed additively manufactured lost core tooling aimed at the aerospace market, however there are very few, cost effective, alternative methods of manufacturing lost core molds. In this study high-impact polystyrene (HIPS) is used as a lost core mold for a composite lattice structure.

MATERIALS AND METHODS

The goal of the study was to provide a proof of concept for the use of an additively manufactured HIPS lost core mold. A consumer grade 3d printer, using 1.75mm diameter HIPS filament , was used to additively manufacture the mold. The part was manufactured from carbon fibre epoxy using single carbon fibre tows which were pre-impregnated with epoxy resin. A suitable 3D printer and all materials and consumables can be purchased for less than €300. The mold was modelled in CAD and imported into Creality Print. The part was printed with a 10% gyroid infill. Once the mold was printed, the prepreg carbon fibre tows were manually wrapped around the tooling. The part was allowed to cure at room temperature after which it was submerged in acetone. The acetone degraded the HIPS and the part was removed from the mold.

RESULTS AND DISCUSSION

The model of the mold, the part layed up prior to mold removal, and the final part are shown in Fig. 1. The study shows that HIPS can successfully be used in the manufacture of lost core molds. This can enable cost efficient, rapid prototyping of complex composite parts, and could be combined with automated composite layup processes such as Automated Tape Placement for more precise layup of composite parts.





Figure 1: Left, Model of tool; Middle, Part layed up on HIPS tool; Right, Final part after removal of HIPS



Abstract

Transmissive Spatial Light Modulators (SLMs) for Discontinuity Generation	
Koliyatan Manamparambil, Raveena, Devaney, Nicholas.	
1. School of Physics, Applied Optics, University of Galway	

INTRODUCTION

The largest telescopes used in astronomy are segmented and errors in segment alignment introduce wavefront discontinuities. This experiment investigates the performance of transmissive SLMs in generating phase discontinuities. For measuring the discontinuity, it utilizes a small circular aperture that is centered on the discontinuity. When the Optical Path Difference (OPD) between the two segments is zero, the PSF is an Airy pattern. As the OPD between the two segments increases, the PSF begins to split into two peaks, with the amplitude of the peaks being equal when the OPD = $\lambda/2$. It is possible to determine the phase difference between the two segments by taking the ratio of the two peaks, and comparing with the ratio for simulated images.

MATERIALS AND METHODS

The setup uses a 532 nm Laser. An aperture of size 10 mm is placed after the Laser. The beam then passes through a linear polarizer (P) at an angle 0^0 with respect to the long axis of the liquid crystal molecules at the input side of the SLM. A transmissive SLM which is placed in the path of the polarised Laser beam used to generate the phase screen and half of the SLM is held with the grey value of 0, the other side varying between 0 and 255 grey levels. An analyser (A) is placed after the SLM which should be rotated until it passes maximum light found to be 60^0 . The light that is passing through the analyzer is focused using a convex lens of focal length 200mm and a microscopic objective onto a CCD camera.



Figure 1 : Optical setup used for experiment

RESULTS AND DISCUSSION

The resulting PSF images for different grey values like 0, 120, 150, 170, 205, and 255 using transmissive SLMs is given in the figure below.



Figure 2: PSF's taken from the Transmissive SLM when two side of the SLM screen were set to grey level differences of 0, 120, 150, 170, 205 and 255.

Transmissive SLMs can be used to model discontinuous wavefronts. However, they do produce much phase change, typically less than a wave, and since they are based on twisted nematic liquid crystals, they produce undesired an amplitude modulation.



Abstract

Sm16, a potential Schistosoma cathelicidin-like immunotherapeutic
Lalor, R. ¹ , Hamon, S. ¹ , Cwiklinski, K. ^{1,2} , Gaughan, S. ¹ , Winrow, D. ¹ , Donnelly, S. ^{1,3} and Dalton, J.P ¹
¹ Molecular Parasitology Laboratory (MPL), Centre of One Health and Ryan Institute, School of
Natural Sciences, University of Galway, Galway, Ireland.
² Institute of Infection, Veterinary and Ecological Sciences, University of Liverpool, UK
³ School of Life Sciences, Faculty of Science, The University of Technology Sydney, Ultimo, NSW,
Australia.

INTRODUCTION

Sm16 is a low molecular weight protein (~16kDa) secreted by *Schistosoma mansoni*, a causative agent of human schistosomiasis. Phylogenetic, structural and functional analysis of Sm16 provides evidence for its inclusion within a family of helminth defence molecules, cathelicidin-like immunomodulators exclusive to trematodes. A synthetic peptide of Sm16 (Sm16_{KS84}) was previously shown to display an immunomodulatory function, however exerted a weak pro-inflammatory response limiting its utility as an immunotherapeutic.

MATERIALS AND METHODS

New synthetic peptide derivatives of Sm16 were designed based on *in silico* analysis of the structural and physicochemical properties of the Sm16 protein. The anti-inflammatory activity of peptides were investigated by stimulating bone marrow derived macrophages with toll-like receptor ligands or the inflammasome activation stimulant, monosodium urate crystals (MSU), and examining differences in cytokine secretions or enzymatic activity in lysates. In addition, to determine if the anti-inflammatory effects observed *in vitro* were translatable in an *in vivo* model of inflammation, peptides were administered therapeutically in a dextran sulfate sodium (DSS) induced colitis model of inflammatory bowel disease in mice.



RESULTS AND DISCUSSION

A shortened synthetic peptide derivative of Sm16 encompassing only the amphipathic helical section of the C-terminus (Sm16_{KS66}) exhibited greater suppressive activity on both pathogen and damage associated inflammatory responses, but also no longer exerted the pro-inflammatory responses like those observed for Sm16_{KS84}. This novel fragment inhibited NLRP3 inflammasome activation, via inhibition of vATPase induced lysosomal acidification and also suppressed bacterial endotoxin activation of macrophages by extracellular neutralisation of the antigen. Moreover, the Sm16_{KS66} peptide retained bioactivity *in vivo*, attenuating the severity of DSS induced colitis. Our findings demonstrate that this small synthetic peptide exhibits potent immunomodulatory properties that are retained *in vivo*, highlighting the immunotherapeutic potential of trematode-derived peptides in the treatment of inflammatory diseases.



Abstract

Cross-Lingual Ontology Matching using Structural and Semantic Similarity	
Banerjee S. ¹ , Chakravarthi B. R. ² , McCrae J.P. ¹	
¹ ADAPT Centre, University of Galway	
² School of Computer Science, University of Galway	

INTRODUCTION

In recent times, deep learning based methods have achieved good results on ontology matching (lyer et al., 2020; Li et al., 2019b). However, these methods are dependent on large amounts of training data which are not available in cross-lingual scenarios. To tackle this challenge we present an unsupervised ontology matching approach for CLOM. The proposed approach uses state-of-the-art text embedding models to embed the concept descriptions into low-dimensional vectors which are then used to compute semantic similarity. Structural similarity between source and target concepts is an integral part of the proposed approach. We leverage the semantic similarity between source and target to learn structural embeddings for each concept in source and target ontologies. The semantic and structural embeddings are then used to calculate a weighted similarity to find equivalent entities in two ontologies. The main contributions of this work can be summarized as follows:

• Our experiments reveal that a weighted combination of semantic and structural similarity achieves performance gains over lexical similarity measures.

• We evaluate our method on 3 language pairs to demonstrate its extensibility.

• The proposed approach does not require manually labeled alignment data and thus is suitable for application in data-scarce scenarios



Abstract

Novel Occupational Exposure Measurement via Passive Tracking Borkowski, S. 1, Conneely, P. 2, House, E 2, Tuohy, B 2, Dr Deegan, B. 1 1 School of Engineering, University of Galway. 2 Dept Medical Physics and clinical engineering, Galway University Hospital

It is documented that Interventionalists face high occupational radiation exposure from to scattered radiation in fluoroscopy procedures [1]. Personal dosimetry is one tool, which is used to mitigate the risks. It is often cited by regulators, that compliance with badge wearing is poor. In addition, it creates an additional burden to medical physicists, who have to perform dose estimation calculations. These calculations are often overestimated, due to poor data on staff exposure time, position, and scatter. This work initially focused on passive location tracking to improve the accuracy of the calculation from a time and position perspective.

Materials & Methods

An Intel RealSense D455 camera was used to monitor each staff member's position throughout procedures. In addition to a standard RGB, this camera uses infrared point clouds to measure distance.

DoseWise provided timestamps and exposure settings. These were used to correlate staff presence during each exposure. Staff identification and labelling was provided by radiographers.

Results

The proposed method tracks the location of staff relative to the radiation source.

The system was proven to measure position to cm resolution.

The system was not affected by occlusion events.

It was not affected by staff infection control PPE.

It can work in low light conditions.

The data can be outputted in CSV format for analysis and presentation.

Conclusion

The system proved that it can be used to accurately and reproducibly track staff position in interventional procedures. Allowing for more accurate dose estimation. Work is ongoing to improve previous scatter measurement to create a one stop solution.

In addition to calculation. The data provided by tracking can be utilised to audit safety culture practice i.e. Time, Distance, Shielding. This works shows that passive tracking can be used to improve radiation safety practices in hospitals.

Acknowledgements

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References

Miranda S. Martinez Lopez, Measurement and Calculations of Radiation Scatter Exposure in Cardiac Angiography, 2023



Abstract

Open Knowledge Base Canonicalization: Techniques and Challenges
<u>Yang, Y.</u>
1. Insight SFI Research Center for Data Analytics, University of Galway
Curated knowledge bases (CKBs) play a fundamental role in both academia and industry. They require significant human involvement to pre-define the ontology and cannot quickly adapt to new domains and new data. To solve this problem, open information extraction (OIE) methods are leveraged to automatically extract structure in the form of non-canonicalized triples <noun noun="" phrase="" phrase,="" relation=""> from unstructured text. OIE can be used to create large open knowledge bases (OKBs). However, noun phrases and relation phrases in such OKBs are not canonicalized, which results in scattered and redundant facts. In order to disambiguate and eliminate redundancy in such OKBs, the task of OKB canonicalization is proposed to cluster synonymous noun phrases and relation phrases into the same group and assign them unique identifiers. Nevertheless, this task is challenging due to the high sparsity and limited information of OKBs. In this paper, we provide an overview and analysis of the techniques used by the main frameworks and discuss the challenges in this topic.</noun>



Ollscoil na Gaillimhe University of Galway

Coláiste na hEolaíochta & na hInnealtoireachta College of Science & Engineering

INNOVATION FOR HEALTH





Abstract

Developmental biology of *Fasciola hepatica*: 3D co-culture using HepG2 spheroids to create mini-livers allows investigation of host-pathogen interactions

<u>Vitkauskaite, A.¹</u>, Cwiklinski, K.², McDermott, E.³, Lalor, R.¹, De Marco Verissimo, C.¹, H. Dehkordi, M.⁴, Thompson, K.³, Owens, P.³, McAuliffe, J.¹, Fearnhead, H.O.⁴, Calvani, N.E.D.¹, Dalton, J.P.¹

¹Molecular Parasitology Laboratory, Centre for One Health, Ryan Institute, School of Natural Sciences, The University of Galway, Galway, H91 TK33, The Republic of Ireland.
²Institute of Infection, Veterinary and Ecological Sciences, University of Liverpool, Liverpool, UK
³Anatomy Imaging and Microscopy (AIM), Anatomy, School of Medicine, The University of Galway,

Galway, H91 TK33, The Republic of Ireland.

⁴Pharmacology and Therapeutics, School of Medicine, The University of Galway, Galway, H91 TK33, The Republic of Ireland.

INTRODUCTION

The helminth parasite *Fasciola hepatica* is a significant cause of animal and human morbidity worldwide. The parasite infects 17 million people worldwide, with 180 million being at risk of infection. Investigations of the parasite's developmental biology are hampered by our inability to culture and propagate juvenile worms *in vitro*.

MATERIALS AND METHODS

HepG2 is a human non-tumorigenic liver cell line with high proliferation rates and epithelial-like morphology. We cultured the infective stage of the parasite, the newly excysted juvenile (NEJ) with HepG2-derived spheroids for 21 days *in vitro* to investigate its development and simulate host-pathogen interactions. We studied parasite development using immunohistochemistry, scanning electron microscopy (SEM), and using antibody probes against two major NEJ proteases, FhCL1 and FhCL3.

RESULTS AND DISCUSSION

We have shown that co-culture with three-dimensional HepG2 cell aggregates (3D spheroids) promotes the survival, growth and development of the newly excysted juvenile *F. hepatica in vitro*. Parasites grown in the presence of HepG2 spheroids, mini-livers, were observed regularly interacting with the spheroids, invading the tissue, indicating the importance of tactile stimuli. Parasites actively feed on and ingest the peripheral cells of the spheroids. The parasites exhibited not only a rapid increase in size and temporal expression of developmental genes, but also extensive development of the gut caecum, musculature, and surface sensory system. Parasites grown with 3D mini-livers mimic *in vivo* parasite-host liver interactions, greatly improving our ability to investigate and understand *F. hepatica*-host biology. This co-culture system has the potential to facilitate the development of new parasite growth and development.



Abstract

Investigation of CDC5L-POLH, a novel fusion gene in cancer
Usmani, A. ₁ , Carty, M. P. ₂
1,2 University of Galway
1,2 University of Galway

Genome instability is a hallmark of cancer, and alterations in key DNA damage repair and tolerance pathways occur in cancer. During replication, specialized polymerases are recruited to bypass unrepaired DNA lesions through a process called translesion synthesis (TLS), facilitating progression. The TLS enzyme Pol η encoded by the human POLH gene on chromosome 6p21, accurately bypasses UV*-induced pyrimidine dimers and can also bypass cisplatin-induced intrastrand crosslinks contributing to cancer chemoresistance. Inherited mutations in POLH cause the rare, sun-sensitive, skin cancer-prone genetic disorder xeroderma pigmentosum variant. Over 500 somatic POLH mutations, including 15 fusion genes, are also reported in cancer genomics databases. Fusion genes, caused by chromosomal rearrangements, can contribute to cancer progression. The CDC5L-POLH fusion gene, formed between POLH and the CDC5L gene encoding an mRNA splicing factor, was identified in stomach adenocarcinoma. CDC5L-POLH encodes an in-frame protein, comprising the Nterminal of CDC5L and C-terminal of Pol η , while lacking the N-terminal catalytic domain of Pol η . However, the role of this fusion gene in cancer remains unexplored. The effect CDC5L-Pol n expression on DNA damage responses and mRNA expression is being investigated using various approaches. Expression of GFP-CDC5L-POLH cDNA in Pol n-knockout and WT MCF-7 cells shows the fusion protein is localised to the nucleus as confirmed by Western blot and fluorescence microscopy analysis. To directly analyse the effect of fusion gene expression in an isogenic human cell system, doxycyclineinducible system is being developed. His-tagged CDC5L-Pol n protein has been isolated from E.coli for protein-protein interaction and structural studies. To generate cells with the CDC5L-POLH genomic rearrangement, RPE1 have been transfected with vectors expressing Cas9 and gRNAs targeting CDC5L and POLH loci on chr6 and targeting will be confirmed using sequencing. This research will shed light on the role of the CDC5L-POLH gene in cancer, offering diagnostic and therapeutic possibilities.



Coláiste na hEolaíochta & na hInnealtóireachta College of Science & Engineering

Use of Synthetic data for Diagnosing Stanford Type B Aortic Dissection

Abaid, A.₁, Farooq, M.A₂, Corcoran, P₂, Ullah, I.₁ 1.School of Computer Science, University of Galway, Ireland 2.School of Engineering, College of Science and Engineering, University of Galway, Ireland

Background

Type B aortic dissection (TBAD) occurs when a tear develops in the descending part of aorta. This tear results in the separation of the inner and middle layers of the aorta, creating a second pathway for blood flow known as a false lumen (FL), which can also obstruct blood flow in the true aortic channel, i.e., the true lumen (TL). The diagnostic and prognostic process of TBAD involves the segmentation of FL, TL, and the false lumen thrombosis (FLT). Manual segmentation of TL, FL, and FLT is challenging and time intensive. Given the low incidence of TBAD, a significant constraint arises from the limited size of the dataset employed for training and testing. This limitation becomes particularly noticeable when dealing with instances of uncommon morphologies, such as FLT, and it hampers the optimal performance of the deep learning model. Since the availability of large-scale labelled data is a contributing factor to the success of deep learning models, there is a significant need to gather data with varying morphologic findings and imaging parameters.

Aims

In this study we aim to enhance the diagnosis and prognosis of TBAD by generating 2D synthetic CTA data using text to image diffusion model and validating the rendered CTA images using quantitative and qualitative methods.

Method

Generation of synthetic CTA data is done by optimal fine tuning of stable diffusion model by incorporating few-shot image learning and low rank adaption (LoRA) model. Rendering of TBAD data with advanced data augmentation based on user specific text prompts was than to achieve high quality synthetic CTA images. Effectiveness of the proposed method was done by statistically analysing the quality and diversity of synthetic images for each class. For this purpose, Frechet Inception Distance (FID) and Multiscale Structural Similarity Index Measure (MS-SSIM). Lastly, to ensure the utility of synthetic images, we trained state-of-the-art (SOTA) model i.e. UNet on real data to evaluate the quality of synthetic CTA images by subjecting them to analysis using our model, examining the presence of features that can be detected by the model.

Results

Results reveal that the output from diffusion model consistently attained MS-SSIM scores closer to those of the original data across nearly all classes. When the synthetic data was subjected to the UNet model trained on real data, successful detection of ROI was achieved for majority of classes.



Figure 1: Real images (first row), synthetic images (second row) and segmentation results predicted by UNet on corresponding synthetic image (third row).



Abstract

Predicting biochemical recurrence in prostate cancer using a novel ceRNA regulatory network
DIGBY, B. 1
_{1,} School of Maths, University of Galway
Biochemical recurrence (BCR) occurs in one-third of prostate cancer patients treated with local therapy and inevitably develops in all patients treated with enzalutamide. Circular RNAs (circRNAs) are covalently closed transcripts involved in cancer pathways and disease mechanisms, harbouring microRNA (miRNA) response element sites within their sequence suggesting a regulatory role within the competing endogenous RNA (ceRNA) network. In this study, we combine prostate adenocarcinoma (PRAD) and enzalutamide-resistant circRNA, miRNA and messenger RNA (mRNA) expression datasets to derive a ceRNA network for effective prediction of BCR in prostate cancer. A prognostic model was constructed using the ceRNA network via Cox regression and stepwise regression in TCGA-PRAD. The linear predictors from the 4-gene prognostic model effectively stratified patients into high-risk and low-risk groups with significantly different BCR outcomes. High-risk patients exhibited unfavourable prognosis and elevated immune infiltration compared to low-risk groups. Moreover, the prognostic model exhibited high prediction accuracy in classifying patients with BCR events in six external validation datasets. This study represents a first-of-kind analysis of circRNA-miRNA-mRNA regulatory networks in prostate cancer and enzalutamide-resistant cells, offering insights into the potential regulatory role of non-coding RNAs in BCR.


Abstract

The Effect of Gap Junction Suppression on the Proliferation of Breast Cancer Cell Lines

<u>Harkin, B.S</u>1, M^cNamara, L.M1, M^cEvoy, E1.

1. Discipline of Biomedical Engineering, University of Galway

INTRODUCTION

Breast cancer is the most common cancer worldwide with gold-standard chemotherapy being a poorly suited treatment option. Gap junctions (GJ) are known to play a crucial role in cell communication and in the context of spheroid growth, have both promoting and inhibitory effects on tumours. The overall aim of this project is to fabricate breast cancer models that reveal the biophysical processes governing tumour growth and resistance to cellular penetration.

MATERIALS AND METHODS

Murine mammary 4T1 and human T47D cells were expanded in their growth media (RPMI supplemented with 10% FBS and 1% penicillin/streptomycin) and maintained at 37°C in a humidified 5% CO_2 environment.

2D Culture: Cells were seeded onto 96-well plates at various seeding densities. Carbenoxolone (CBX) concentrations were prepared and added to the cells at day 3.

3D Culture: Cell encapsulating gelatin hydrogels (1.1 kPa) were developed by crosslinking equal volumes of 9% gelatin and nano-Hydroxyapatite (5.5% v/v) with microbial-transglutaminase (mtgase) of 1% w/w concentration. Cell number was kept at 3×10^6 cells/hydrogel.

All groups were cultured for 7 days. Samples were then fixed and permeabilized with 0.5% Triton-X in PBS. Cells were stained with phalloidin-FITC and DAPI. Samples were also incubated overnight with primary antibody Connexin-43 (16825305, Fisher), diluted at 1:1000. After washing with BSA, samples were incubated with secondary antibody, goat anti-mouse Alexa 488 (A11029, Invitrogen), at 1:200, for 1hr protected from light. 2D samples were assessed for proliferation. 3D samples were assessed for tumour spheroid size and Cx-43 expression. Imaging was carried out using a Confocal Microscope (FV3000) and processed using ImageJ software.



RESULTS AND DISCUSSION

Both cell lines treated with CBX resulted in a decreased proliferation when assessed on day 7. Anti-Cx43 showed ample expression of gap junction concurrent to the number of viable nuclei present in the spheroids. Understanding the role of GJs, particularly the Cx43 protein, in influencing tumour growth will drive our understanding of why these channels might both supress and increase growth.

Figure 1 Pilot Study showing the effect of CBX drug treatment on T47D Cell line in 2D Culture.



Abstract

Heterogeneous glycosylation of proteins from *Fasciola hepatica* invasive stage reveals higher complexity in parasite-host interactions

De Marco Verissimo, C.¹, Cwiklinski, K.^{1,2}, Nilsson, J.³, Mirgorodskaya, E.³, Jin, C.³, Kilbane, T.¹, Karlsson, N. G.⁴, Dalton, J. P.¹

¹ Molecular Parasitology Laboratory, Centre for One Health and Ryan Institute. University of Galway.

 ² Institute of Infection, Veterinary and Ecological Sciences, University of Liverpool, UK.
 ³ Proteomics Core Facility, Sahlgrenska Academy of Science, University of Gothenburg, Gothenburg.
 ⁴ Department of Life Science and Health, Faculty of Health Science, Oslo Metropolitan University, Oslo.

Fasciola hepatica uses glycosylated excreted-secreted (ES) and surface molecules to interact with host cells and tissues, and to evade damage caused by cellular and immune responses during host invasion. Despite the unknown glycosylation state of many of the ~100 different proteins found in the ES of the immature invasive stage of F. hepatica (NEJs), several are extensively used as diagnostic and vaccine targets. To develop more effective strategies against fascioliasis, information on the glycosylation profile of individual NEJs proteins is critical. In this study, we used a combination of glycan, glycopeptide, and proteomic analyses, along with bioinformatics tools, to identify the glycosylation status of individual F. hepatica NEJs proteins. Our results identified 123 glycoproteins in NEJs extracts, 71 of which were in the ES. We mapped 3 glycopeptides and all the 1,696 N-glycan forms and 37 O-glycan forms to their respective protein and glycosites, revealing a high degree of heterogeneity in the glycosylation of F. hepatica NEJs proteins (i.e., in average, 14 glycan forms can be used to modify each glycoprotein). Unique glycan motifs, such as PC and multi-PC terminals, and xylosylated O-glycan cores, were found in 25 distinct NEJs glycoproteins, including cathepsin peptidases B and L, which are well-known vaccine and diagnostic targets. Furthermore, many parasite proteins carried highly truncated N-glycans and structures with undefined linkages that could not be assigned (i.e., HexNAc2Hex₄dHex₁), and the roles of which in parasite infection are largely unknown. These structures are present in excreted-secreted or predicted membrane-bound glycoproteins, suggesting that they play key roles in NEJs interactions that command host invasion. Our findings demonstrate that F. hepatica NEJs generate great protein variability via glycosylation, and that the larvae extracts are far more complex than anticipated by proteomic analysis. This data provides a foundation for improving diagnostics and vaccine development to control fascioliasis.



Abstract

Experimental Characterization and Computational Modelling of Brain Tissue

Sheridan, C., Concannon, J.

Biomedical Engineering, College of Science and Engineering, University of Galway

INTRODUCTION: The damage mechanism for concussion in unknown, and diagnosis hinges upon the lack of evidence of damage on MRI/CT scanning [1]. Though the impact of individual concussions cannot be quantified clinically, it has been seen that repeated concussion contributes to neurodegenerative conditions such as Parkinsons, CTE and Dementia [2]. Many publications refer to "brain tissue" as a homogenous material, neglecting regional and grey/white matter variance. As a first step in understanding the response of brain tissue to impact, this study performs regional mechanical testing on the grey and white matter of ovine brain tissue, and investigates the efficacy of inbuilt constitutive laws in capturing the experimental trends.

MATERIALS AND METHODS: Due to ethical and logistical limitations, ovine brain was used, being dissected to isolate samples of each matter from each lobe. Unconfined compression, unconfined tension, cyclic (tension and compression), and shear mechanical loading was carried out for each tissue type and location. Compression, tensile, and shear tests were performed up to 50% strain, while cyclic testing was performed between -1% and 2.5% strain, with all testing performed at a load rate of 25%/s. Once normalised and averages found, compression and tension data were conjoined, to find the regional and overall average responses. Using this, Mooney-Rivlin Parameters were fit to the grey matter data for computational modelling of the grey matter as a whole.

RESULTS AND DISCUSSION: Figure 1 below details the regional variance in the mechanical response of grey and white

matter, where the computational model can be seen to overpredict regional stress in compression by 75%, and underpredict by 30%, while for tension it can underpredict stress by up 65% to and can overpredict by up to 72%. Stiffness up to 10% in white matter tension can be seen to varv significantly, with initial moduli of ~0.85 kPa, 0.39 kPa and 0.14 kPa for the occipital region, corpus callosum, and computational





respectively. This level of underprediction of stress, in a clinically relevant strain region [3] show that one homogenous constitutive law is insufficient for predicting the properties of brain tissues. Morphological differences have been noted microstructurally between grey and white matter samples under Hematoxylin & Eosin and Cresyl Violet staining which may provide insight in the macroscopic differences in behaviour between the tissues.

These regional variances in mechanical properties will have a marked effect on the transmission of mechanical loads throughout the brain in concussion-type loading modes, affecting the prediction of physiological damage.

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model

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Abstract

Shamavu, D. 1
1. University of Galway - School of Science

Abstract

DNA replication is a fundamental process in which a cell duplicates its genetic material to pass on to daughter cells. It occurs during cell division and involves the unwinding of the DNA double helix, followed by the synthesis of two new complementary strands. However, DNA is prone to damage from various sources such as chemicals and radiation. This damage can lead to mutations if not repaired properly, potentially leading to the development of cancer. Cells have intricate repair mechanisms to correct these errors, ensuring the fidelity of genetic information and maintaining cellular integrity.

BRCA1 is a crucial gene associated with an increased risk of breast and ovarian cancer when mutated. It encodes a protein involved in repairing damaged DNA that can arise from problems encountered during DNA replication. Individuals with a mutated BRCA1 have a significantly higher susceptibility to developing cancer. BRCA1 mutations impair the cell's ability to repair DNA damage properly, leading to the accumulation of genetic errors and the potential for uncontrolled cell growth. Recent studies, including a genome-wide loss-of-function screen conducted in the Santocanale lab suggests that CDK8 targets proteins involved in DNA damage repair, including BRCA1. However, CDK8, and its activating partner Cyclin C, have known roles in transcription but no well-known roles DNA replication and DNA repair. CDK8 has a paralog named CDK19 with similar structure and function. CDK19's activity is also regulated by Cyclin C.

The aim of my project is to understand CDK8/19's role in DNA regulating DNA damage repair pathways using its potential link to BRCA1. By understanding CDK8's role in detail, it will provide profound implications for cancer prevention, detection, and treatment, including targeted therapies.



Abstract

Advancing Cancer Therapy: The Power of nanoMOFs for Enhanced Drug Delivery <u>McHugh, D. a</u>, Winterlich, M. a, Dwyer, R. a and Papatriantafyllopoulou C. a aSchool of Biological and Chemical Sciences, College of Science and Engineering, University of Galway, H91 TK33 Galway, Ireland.

In cancer research, there is a pressing need for innovative drug delivery systems (DDS) because current APIs on the market (e.g. doxorubicin (DOX)) experience poor bioavailability and lack cancer-targeting abilities resulting in adverse effects and systemic toxicity. Additionally, current DDSs (e.g. dendrimers, micelles) face poor drug loading, toxicities and early-leakage of the drugs. The quest for novel DDS is driven by the urgency to enhance therapeutic efficacy while minimising side effects. ^[1-3]

In this work, we will discuss a novel nanoMOF (OnG8) with a great potential to combat the above issues. NanoMOFs have demonstrated low toxicity, high drug loading and a controlled drug release mechanism. These advancements represent a transformative shift in cancer therapy, holding the potential to revolutionise chemotherapy. OnG8 consists of of a zinc cluster and a multitopic elongated carboxylate linker, ([Zn₄O(L'H₃)]n). It was synthesised to obtain <350 nm average octahedral nanoparticles. The elongated nature of the organic resulted in a highly microporous MOF with a surface area of 5000 m²/g and pore sizes of 1.9 nm. The highly porous nature of OnG8 resulted in high doxorubicin loading after 5 days (1.1 g DOX/g OnG8). Drug release studies in PBS at various pH's and displayed an acidic pH-responsive drug release. The structure, drug delivery, and cytotoxicity properties of OnG8 will be discussed in detail.



Figure 1 SEM image of OnG8 (left) and Absorption of DOX by OnG8 (right)

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Abstract

NOVEL PATIE	NT-SPECIFIC BIVENTRICULAR HEART MODEL INTEGRATING PSEUDO-FLUID DOMAINS	
	<u>Senthil, D1</u> , Concannon, J1, McGarry, P1	
1.	Discipline of Biomedical Engineering, School of Engineering	

INTRODUCTION

We propose a novel FE-based approach to modelling a biventricular heart. We utilize custom userdefined materials (UMATs) to model the active contractile myocardium and we develop novel "pseudofluid domains" to model blood in the right (RV) and left (LV) ventricles without resorting to Fluid-Structure Interaction (FSI) simulations. This novel approach allows for the simulation of a cardiac cycle in 30 minutes, 3-4 orders of magnitude faster than FSI heart models.

MATERIALS AND METHODS

Patient-specific biventricular meshes are developed from MRI images (Fig. 1A). Our myocardium material model incorporates passive isotropic and anisotropic components and actively contracting cardiac myocytes [1]. Fibre directions are prescribed using the Laplace-Dirichlet Rule-Based (LDRB) algorithm [2]. Our novel "pseudo-fluid domain" approach is used to determine ventricle volume and pressure changes in response to myocardial contraction. During systole, pressure and volume changes in each ventricle are governed by a Windkessel formulation.

RESULTS AND DISCUSSION

The fibre orientations produced by the LDRB algorithm (Fig. 1B) accurately resemble those observed invitro and allow our model to accurately demonstrate apicobasal shortening and twist (Fig. 1C). Fig. 1D shows the PV loops computed from a 7-cardiac cycle simulation of Inferior Vena Cava Occlusion (IVCO). The model correctly predicts reductions in end-systole (ES) and end-diastole (ED) pressure and stroke volume (SV) in both ventricles over a series of cardiac cycles. Finally, the total computing time for this 7-cycle simulation was 3.5 hours, orders of magnitude faster than traditional FSI approaches.



Figure 1: (A) Construction of 3D patient-specific meshes from MRI stacks; (B) Fibre orientations given by the LDRB algorithm; (C) Contour plots showing computed myocardium active stress;
(D) Computed PV loops for the LV (red) and RV (blue) over a 7-cycle simulation of IVCO.

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Abstract

SCORPIONISM: INSIGHT FROM A ONE HEALTH PERSPECTIVE	
Leonard, D ^{1,2} , Boyd, A ¹ , Dugon, M.M ² .	
 Pathogenic Mechanisms Research Group, School of Natural Sciences, University of Galway Venom Systems and Proteomics Lab. School of Natural Sciences. University of 	
Galway	

INTRODUCTION

1.2 million people are stung by scorpions every year resulting in over 3,250 deaths. Scorpionism disproportionally impacts the most vulnerable demographics in developing nations. 90% of deaths involve children under 15 from poor and rural backgrounds. Long term effects of scorpion envenomings have not been systematically studied but cases in medical reports include organ defects and severe infections.

Regarding bacterial infections, the microbial communities of the scorpion sting apparatus are vastly understudied. Fungi which are also seen in post envenoming infections are often overlooked until a mass infection occurs.

The aim of our work is to ascertain the microbiome of the scorpion sting apparatus and understand the relationship between the microbes within the venom system and those in their environment with a focus on the ability of scorpions to act as reservoirs for pathogens that could transfer to humans during envenomings.

RESULTS

Scorpio mogadorensis, the Moroccan Brown scorpion, is the model organism within the study. Samples of venom system swabs, stinging apparatus and soil samples from three habitats were collected from the Tiout Oasis in Morocco. Bacterial isolates were cultured from these samples on a range of media. The samples will also be used for rRNA microbiome analysis as culturing fails to encompass the full microbiome. To date 111 bacterial and 8 fungal isolates have been cultured from the scorpion venom system.

DISCUSSION

Using the rRNA microbiome data, we aim to show if the microbiome of scorpions is sexspecific, specimen-specific or habitat-specific. Particular interest is placed on microbes classified as ESKAPE pathogens. Data will be investigated from the perspective of microbial reservoirs, human interaction and the risk of stings transmitting pathogenic microbes to humans during envenoming.



Abstract

Towards Explainable Deep Learning in Oncology: Integrating EfficientNet-B7 with XAI techniques for Acute Lymphoblastic Leukaemia Muhammad, D. 1 1. School of Computer Science

Acute Lymphoblastic Leukaemia (ALL), presents a significant threat to human health due to its rapid progression and impact on the body's blood-producing system. The accurate diagnosis derived from thorough investigations plays a crucial role in formulating effective treatment plans that can influence the likelihood of patient recovery. In the pursuit of refining diagnostic accuracy, diverse Machine Learning (ML) and Deep Learning (DL) approaches have been employed, demonstrating remarkable performance in analyzing intricate biomedical data for identifying ALL. However, the complex nature of these algorithms often makes them difficult to comprehend, posing challenges for patients, medical professionals, and the wider community.

To address this issue, it is imperative to elucidate the functioning of these ML/DL models, fostering trust and providing users with a clearer understanding of diagnostic outcomes. This paper introduces an innovative framework for ALL diagnosis by incorporating the EfficientNet-B7 architecture with Explainable Artificial Intelligence (XAI) methods. Firstly, the proposed model accurately classified the ALL using microscopic images and achieved performance scores of AUC 96.04%, mAP 94.45%, Accuracy 97.13%, Precision 99.32%, Recall 92.42% and F1-score 95.75%. Secondly, the XAI approaches namely LIME, Grad-CAM and Grad-CAM++ were applied to explain the proposed model decision.

Our contributions to pioneering the use of EfficientNet-B7 in conjunction with XAI for the diagnosis of ALL, set a new benchmark for trust and transparency in the medical field.



Abstract

RoboHeal: Development of a soft robotic drug delivery system to improve treatment of diabetic foot ulcers
Wallace, E.W. _{1,2,3} , O'Dwyer, J.4, Duffy, G.P. _{3,5} , Cameron, A.2, Dolan, E.B.1,3.
 Biomedical Engineering, School of Engineering, University of Galway, Galway, Ireland FeelTect, Páirc na Meán, Bohoona East, An Spidéal, Co. Galway, Ireland CÚRAM, SFI Research Centre for Medical Devices, University of Galway, Galway, Ireland Pharmacology, School of Medicine, University of Galway, Galway, Ireland Anatomy and Regenerative Medicine Institute (REMEDI), School of Medicine, College of Medicine Nursing and Health Sciences, University of Galway, Galway, Ireland
INTRODUCTION Diabetic foot ulcers (DFU) are a complication of diabetes mellitus with a worldwide incidence between 9.1 to 26.1 million. The estimated cost of treating DFU is \$1.38 billion per year with current treatment options including wound debridement, wound dressings, topical antibiotics or antiseptics, compression therapy, offloading techniques, and surgical interventions. Despite these treatments, approximately 20% of individuals with a DFU will undergo lower-extremity amputations. Further, 10% of individuals with DFU will die within 1 year of diagnosis. The management of DFU requires a multidisciplinary approach and so this research aims to combine soft robotics with mechanoresponsive hydrogels to achieve spatiotemporal release of angiogenic growth factors on the wound surface and then apply negative pressures to promote granulation to encourage healing of DFU (Fig. 1).
(A) (B) (C)



Figure 1: Schematic of the RoboHeal to encourage healing of diabetic foot ulcers. (A) Pneumatic actuation of soft robotic device to compress hydrogel and spatiotemporally release angiogenic growth factors. Application of negative pressure using soft robotic device to encourage (B) macro deformation, and (C) micro deformation.

METHODS

Design and fabricate soft robotic devices consisting of an actuation reservoir and therapeutic reservoir (Fig. 1). Complete wound healing assays to determine dose and timing of vascular endothelial growth factor (VEGF) and platelet derived growth factor (PDGF) to stimulate angiogenesis. Optimise hydrogel formulation to electrostatically interact with VEGF and PDGF and optimise the actuation regime in *in vitro* drug release studies to release predetermined amounts of VEGF/PDGF to stimulate angiogenesis in future rodent wound healing models.



Abstract

Predicting and Optimising Pulsed Field Ablation Sizes with Design of Experiments in In Vitro Samples	
<u>Dunne, E_{1,2,3},</u> Baena-Montes, J. M. _{3,4} , Donaghey K. ₅ , Clarke C. ₅ , Kraśny, M. J. ^{1,6} , Amin B. <u>1</u> O'Halloran, T. ₅ , Quinlan L. R. _{3,4} , Elahi A. <u>1,2,6</u> , and O'Halloran M. <u>1,2,3</u>	. <u>,2,3</u> ,
 Translational Medical Device Lab (TMD Lab), University of Galway, Galway City, Ireland Electrical & Electronic Engineering, College of Science and Engineering, University of Galway, Galway City, Ireland School of Medicine, University of Galway, Galway City, Ireland Physiology and Cellular Physiology Research Laboratory, CÚRAM SFI Centre for Research in Medical Devices, School of Medicine, Human biology building, University of Galway, Galway, City, Ireland 	l
 AuriGen Medical, GMIT Innovation Hubs, Galway City, Ireland Smart Sensors Lab, Lambe Institute for Translational Research, School of Medicine, University of Galway, Galway City, Ireland 	

INTRODUCTION

Atrial Fibrillation (AFib) is a common cardiac arrythmia that is becoming more frequently treated with cardiac catheter ablation. While typically carried out by thermal methods, pulsed field ablation (PFA) is a recently-adapted technology for the procedure whose method of ablation is non-thermal, reducing risk of collateral damage. The ablation size of PFA is dependent on electrode and waveform parameters (factors). In this work, the statistical method of Design of Experiments (DoE) is utilised for the design and optimization of a PFA device for AFib.

MATERIALS AND METHODS

A full-factorial design was used to analyse the four factors of input voltage, electrode spacing, electrode width, and on-time and their interactions. A custom probe, designed for a 6-well plate, was formed with copper electrodes (height of 4.5 mm). Monolayers of human cardiomyocyte cell line AC16 were grown in 6-well plates and then, ablated with the custom probe. The cell death was assessed two hours post-ablation using the live/dead assay and by imaging monolayers on the EVOS M7000 Imaging System microscope. The ablation area was calculated in ImageJ. The results were then feed to the Minitab and an empirical model formed to predict and optimize the ablation size responses.

RESULTS AND DISCUSSION

The input voltage, the electrode spacing, and the on-time were found to significantly affect the ablation size, aligning with the literature. The results also found that two-factor interactions played a significant role and need to be account for in modelling. An accurate empirical model (< 2.1% error in the measured area) was determined for prediction and optimisation of ablation sizes. The findings and the strong predictive model developed highlight that the DoE approach can be used to help determine PFA device design, to optimize for ablation size, and to help inform device design to tackle specific cardiac arrhythmias.



Abstract

Fasciola hepatica Enolase, a glycolytic enzyme exposed on the newly excysted juvenile (NEJ) tegument: a surprising target for vaccine development.

<u>O'Kelly, E.</u>¹, Cwiklinski, K.^{1.2.}, De Marco Verissimo ,C.¹, Lopez, J.¹, Flaus, A.³, Vitkauskaite, A.¹ Dalton, J.P.¹, Lalor, R.¹

¹Molecular Parasitology Laboratory, School of Natural Sciences University of Galway. ²Institute of Infection, Veterinary and Ecological Sciences, University of Liverpool, UK. ³Centre for Chromosome Biology, School of Natural Science, University of Galway.

INTRODUCTION

Enolase is a 47 kDa enzyme involved in the reversible conversion of D-2-phosphoglycerate (2PGA) to phosphoenolpyruvate (PEP) in glycolysis and gluconeogenesis. This is also an enzyme of potential immunomodulatory importance in the early infection and migratory stages of the trematode parasite *Fasciola hepatica*, and, therefore, a putative target for vaccine development. The present study was performed to obtain biochemical, molecular and biological data about the FhEnolase (*F. hepatica* enolase) that may support its role in host-parasite interaction in the parasitic infection, fasciolosis.

MATERIALS AND METHODS

For that purpose, we produced a functional enzyme by expressing the recombinant form of FhEnolase in an *E. coli* expression system. FhEnolase purified using His-tag affinity purification takes on a dimeric structure of ~94 kDa, as found in other species, when analysed by size exclusion chromatography and enzymatic activity assays. Immunoblotting and confocal microscopy was used to localize the protein in parasite extracts and tissues. Finally, we vaccinated sheep with a recombinant cocktail containing FhEnolase and three other *F. hepatica* metabolic enzymes.

RESULTS AND DISCUSSION

The recombinant enolase is enzymatically functional only as a dimer, and not in its monomeric form. Immunoblotting studies of adult worm extracts indicate that the enzyme is present in the tegument and the excretory/secretory products of the parasite which supports its key role at the host-parasite interface. Confocal immunolocalisation studies of the protein in newly excysted juveniles (NEJ) show that it is expressed on its surface and therefore exposed to antibody binding. Vaccine studies in sheep indicates that while this vaccine did not reduce adult fluke or egg burdens, remarkably, the vaccinated sheep exhibited a noticeable increase in weight. This observation encourages further studies on metabolic enzymes and their possible exploitation as vaccines for parasite infections.



Abstract

Rational design of gold(III)-glycoconjugates as antiviral agents against SARS-CoV-2 Brescia, F., a Ronconi, L.*a aUniversity of Galway, School of Biological and Chemical Sciences, Galway (Ireland);

First identified in Wuhan in December 2019, the Coronavirus Disease 2019 pandemic has been causing a major global health emergency which undoubtedly exposed the fragility of the current globalized society. Remarkably, it was the third recent coronavirus-related outbreak after SARS-CoV (2002) and MERS-CoV (2012), thus highlighting the urgent need for dedicated antiviral therapeutics,[1] not an easy task given their extremely low approval rates.[2] Although substantial efforts in drug design and repurposing have been undertaken, to date only a few drugs have been officially approved for the treatment of COVID-19 infection.[3]

In this context, metal derivatives are generally under-represented in the compound libraries used for screening in drug discovery campaigns, despite the growing evidence of their role in medicinal chemistry. On account of the aforementioned considerations, based on solid encouraging preliminary results recently obtained in our group, [4] we here report on the design of monosaccharide-containing gold(III)-based derivatives as antiviral agents against Severe Acute Respiratory Syndrome Coronavirus-2 (SARS-CoV-2). The goal is to generate non-toxic gold-glycoconjugates to be taken up by coronavirus-infected cells and, once internalized, capable of acting as potent inhibitors of specific SARS-CoV-2 target proteins, such as the Papain-like Protease (PLPro). This protease not only orchestrates key processes in viral reproduction but also plays a strategic role in subverting the host's immune response upon viral infection. Furthermore, the conserved nature of PLPro across the Coronavirus family suggests that targeting this protease may offer a broad-spectrum solution against current and future coronavirus threats.[5]

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Abstract

Mesenchymal stem cell extracellular vesicle attenuate dendritic cell maturation.
Buckley, F. 1
1 REMEDI, Regenerative Medicine Institute, University of Galway

In inflammatory states, dendritic cells infiltrate bone tissue and activate T cells, increase osteoclast differentiation, and subsequently increase bone resorption and destruction. Therefore, the control of dendritic cell maturation is imperative to potentiate repair. The concept of mediating tissue regeneration using transplanted mesenchymal stem cells was primarily based on the early hypothesis that the cells would engraft and differentiate, to replace damaged tissue. However, low engraftment rates and poor survival remain a barrier for exploitation of the multi-potency of mesenchymal stem cells. Despite this, tissue regeneration is still potentiated. These observations gave rise to the developed hypothesis that mesenchymal stem cells facilitate tissue regeneration via a paracrine method, through secretion of soluble factors and extracellular vesicles. Extracellular vesicles are secreted membrane bound nano-vesicles that contain proteins, lipids, micro ribonucleic acid (miRNA), messenger RNA (mRNA), noncoding RNA (ncRNA), deoxyribonucleic acid (DNA), and RNA. Extracellular vesicles are found in most biological tissues and are involved in cargo transfer between cells. It is hypothesized here that mesenchymal stem cell extracellular vesicles are phagocytosed by dendritic cells, and this subsequently attenuates dendritic cell maturation. To test this hypothesis, extracellular vesicles were isolated from the conditioned media of the D1 ORL UVA mesenchymal stem cell line. Immature dendritic cells were differentiated from C57BL/6 bone marrow monocytes in the presence of GM-CSF. Dendritic cell maturation was induced via lipopolysaccharide (LPS) and CpG oligonucleotide stimulation. Mature dendritic cells were subsequently treated with mesenchymal stem cell extracellular vesicles and maturation was assessed via flow cytometry and cytokine analysis. Results show that mesenchymal stem cell extracellular vesicles are phagocytosed by dendritic cells, and this subsequently reduces the surface marker expression of CD80, CD83, CD86, CD40, MHC II and CCR7 on LPS CpG oligonucleotidestimulated dendritic cells. Secretion of inflammatory cytokines from these dendritic cells is also reduced post-extracellular vesicle treatment.



Abstract

Novel molecular assays for detection of the opportunistic pathogen *Kalamiella piersonii*. Faherty, M.¹, Morton, J.¹, Darcy, G.¹, Chueiri, A.¹, Carolan, S.¹, Miliotis, G.^{2,3}, McDonagh, F.^{2,3}, Singh, N. K.⁴, Venkateswaran, K.⁴, Smith, J. T.¹, O'Connor, L.¹.

1. Molecular Diagnostics Research Group, University of Galway, Galway, Ireland.

- 2. Antimicrobial Resistance and Microbial Ecology Group, School of Medicine, University of Galway, Galway, Ireland.
 - 3. Centre for One Health, Ryan Institute, University of Galway, Galway, Ireland.
- 4. Biotechnology and Planetary Protection Group, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, United States.

INTRODUCTION

Kalamiella piersonii is an opportunistic pathogen recently implicated in human infections including bacteremia and kidney stone disease. The organism was first isolated from surfaces on the international space station (ISS). Isolates have been reported as multidrug resistant and have the ability to survive in hostile environments. To date there have been no reports of molecular assays which can reliably detect this organism. In this work we aimed to develop both a specific real-time PCR with good analytical sensitivity and a LAMP assay for rapid, reliable detection of the organism.

MATERIALS AND METHODS

Comparison of whole genome sequences from *K. piersonii* isolates revealed that the malate dehydrogenase gene was highly conserved across the isolates analysed but sufficient sequence variability was observed in the gene in closely related organisms such as Pantoea and Mixta species. This allowed design of primers and Taqman Probes for a real-time assay together with the design of a isothermal LAMP assay. *K. piersonii* isolates including those available from the ISS were tested along with other organisms from the order Enterobacterales.

RESULTS

A real-time PCR assay for the detection of *K. piersonii* was developed. The assay specifically detected only *K. piersonii*. No cross reaction was observed with the closely related organisms tested. The limit of detection of this real-time PCR assay was approximately 10 copies of target per reaction. Likewise, the new LAMP assay showed specificity for *K. piersonii*.

CONCLUSION

A real-time PCR assay for the specific detection of the opportunistic pathogen *K. piersonii* was developed. Additionally, a rapid LAMP assay was developed. The real-time PCR assay has potential to be utilised clinical settings, while the LAMP assay offers the possibility to achieve detection in a low complexity environment with a rapid turnaround time.



Abstract

Immunomodulatory Effect of Mesenchymal Stem Cell-Derived Extracellular Vesicles on

Dendritic Cells

<u>Kimingi.HW¹</u>, Buckley.F², Contereras.KP², Brennan.MÁ^{1,2}

¹Biomedical Engineering, School of Engineering, College of Science and Engineering, University of Galway, Galway, Ireland

²Regenerative Medicine Institute (REMEDI), School of Medicine, College of Medicine, Nursing and Health Sciences, University of Galway, Galway, Ireland

INTRODUCTION

Dendritic cells (DCs) are professional antigen-presenting cells (APCs), forming an integral part of our immune responses as they link the innate and adaptive immune systems. The integration of different signals by DCs, like the cytokine milieu at the inflammation site, may determine the activation of DCs to either tolerance (tolerogenic DCs) or immunogenic DCs. In a physiological condition, the DCs are absent from the surrounding bone marrow matrix and bone tissue. However, DCs have been reported in the synovium's active lesion site in rheumatoid arthritis (RA) and aggregate with T-cells into the periodontal lesion tissue to destroy the periodontal bone tissue on oral gingival tissue. This suggests that DCs may indirectly influence inflammation-related bone loss by activating T cells. It has been shown that mesenchymal stromal cells (MSCs), and more recently their secretome, including extracellular vesicles (EVs), can modulate the immune system. This study investigates the influence of MSC-EVs' potential to modulate dendritic cell differentiation and activation.

MATERIALS AND METHODS

MSCs were cultured on tissue culture plastic in EV-depleted media for 48 hours. EVs released by the MSCs were isolated using size exclusion chromatography (SEC). Isolated EVs were treated on monocyte-derived dendritic cells, and surface markers of dendritic cells were analysed using flow cytometry.

RESULTS AND DISCUSSION

Preliminary results from this study show that the MSC-derived EVs inhibit the differentiation of dendritic cells. Specifically, there was a significant reduction in the expression of MHC-II, CD11c, and CD86 surface markers. Output from this study will expound on strategies to target during the bone healing process with the aim of immunomodulation to help lessen the burden that comes with inflammation-induced bone loss.



Abstract

Oligopeptide-modified oligonucleotides as targeted therapeutics for ESKAPE pathogens
<u>Kelly, J.B.1,</u> O'Flaherty, S.2, Reddington, K.3, O'Gara, J.P.3, Myers, E.3, Murphy, P.3, Devocelle, M.2, Zeden, M.S.1
 School of Biological and Chemical Sciences, Zeden Lab, College of Science and Engineering, University of Galway. Department of Chemistry, Royal College of Surgeons Ireland, Dublin. School of Biological and Chemical Sciences, College of Science and Engineering, University of Galway.
INTRODUCTION
Antimicrobial Resistance (AMR) is a leading global threat to public health, that must be counteracted by the development of novel therapeutics. The ESKAPE group consists of 6 multi- drug resistant pathogens, which are so-called due to their ability to 'escape' our current arsenal of antimicrobial therapeutics. The members of this group are either high or critical priority in the search for novel antimicrobial therapeutics according to WHO and CDC.

Antisense oligonucleotides (ASOs) are RNA therapeutics that can hybridise to a target gene and prevent it from being transcribed **(Fig 1)**. For my PhD project, I aim to identify genes that are required for resistance in the ESKAPE pathogens and target them with ASOs, to resensitize them to existing antibiotics.

MATERIALS AND METHODS

Preliminary bioinformatic analysis using ResFinder has been carried out to characterise the ESKAPE strains used. Antibiotic susceptibility testing has been carried out using disk diffusion assays and minimum inhibitory concentrations (MICs) determined using several antibiotic classes according to CLSI guidelines to establish the current resistance profiles. Fmoc solid-phase peptide synthesis is used to create peptides with linkers to be used as a cargo for the delivery of ASOs into cells.

RESULTS AND DISCUSSION

Susceptibility tests revealed highly resistant strains such as *A. baumannii* (NCTC 13302). The genes responsible were found through bioinformatics analyses using ResFinder, BLAST, Kegg, and ClustalW and evaluated as targets for ASOs. Folding of potential targets will be assessed using MFold and Pymol4RNA to ensure capability for binding ASO targets.

pVec-azide was synthesised, and will be evaluated using the ESKAPE strains for its ability to pass through the cell membrane using confocal microscopy. Additional peptide synthesis will be undertaken to determine appropriate peptide composition for cargo of ASOs into Gram-negative vs Gram-positive species.



Coláiste na hEolaíochta & na hInnealtóireachta College of Science & Engineering





Abstract

 Identification and analysis of transcriptomic changes in MSCs from people with type 2 diabetes mellitus

 Wang, JY.¹, Ó Broin, P.^{*2}, Whysall, K.^{*1}, Colman, C.^{*1}

 1. School of Medicine, College of Medicine, Nursing and Health Sciences, University of Galway, Ireland

 2. School of Mathematical & Statistical Sciences, College of Science and Engineering, University of Galway, Ireland

 * These authors jointly directed this work

INTRODUCTION

Type 2 diabetes mellitus (T2DM) is a chronic disease associated with elevated blood sugar levels (IDF Diabetes Atlas), often leading to osteopathy, characterized by reduced bone mass and increased mineral density. T2DM has been linked to suppressed quantities of osteogenic bone marrow mesenchymal stem cells (MSCs), which are known for their diverse functions and potential in tissue regeneration and disease treatment (PMID: 17575306).

Despite advancements in understanding MSC biology through single-cell RNA sequencing (scRNA-seq), challenges remain in clustering MSC subpopulations and handling data noise (PMID: 37474525). Deconvolution methods have emerged to improve the utility of bulk RNA-seq data by extracting cell type proportions and gene expression profiles. Our study aims to identify MSC subpopulations using scRNA-seq data as reference for deconvolution, followed by comparative transcriptional analysis between T2DM and Non-T2DM individuals. We seek to identify therapeutic targets within this context.

MATERIALS AND METHODS

High-throughput gene expression datasets related to human MSCs were retrieved from GEO database. Gene expression matrices were generated through bulk RNA-seq analysis, involving Trimmomatic for trimming and filtering, followed by alignment to a reference genome using STAR and HTSeq (PMID: 25260700; 24695404; 23104886). MSC subpopulations within the MSCs scRNA-seq data were identified by maker gene expression according to the literature by using Seurat R package (PMID: 37231261), enabling deconvolution in the next analysis step.

RESULTS AND DISCUSSION

Four public available datasets were included in this study. Visualization of the single-cell transcriptomes unveiled the complexity of MSCs' subpopulation. Furthermore, the MSC subpopulations in the MSCs scRNA-seq data were identified based on various transcriptome expression using marker gene from the existing literature. These findings significantly contribute to our comprehension of MSC biology, paving the way for subsequent deconvolution work to compare transcriptional changes of MSC as a result of T2DM.



Abstract

Predicting Muscle Age and Identifying Aging-Related Genes from Gene Expression Data Guerrero-Vazquez, K. 1, Qin, H. 2, O'Broin, P. 1, Goljanek-Whysall, K. 1 1 University of Galway, 2 University of Tennessee at Chattanooga

Understanding the molecular mechanisms underlying aging is essential for developing targeted interventions to mitigate age-related diseases. While recent advancements have employed omics analyses to identify signature genes of various age-related conditions, skeletal muscle aging remains relatively underexplored.

We present a deep learning approach to predict the age of individuals based on gene expression data from human *vastus lateralis*, while identifying key genes associated with muscle aging. We identified genes implicated in well-known aging mechanisms such as inflammation, cell proliferation, and autophagy, intersecting with genes previously published as differentially expressed in sarcopenia.

Our data collection integrates expression data from 19 microarray projects and 12 RNAseq experiments, totaling more than 900 samples from different countries. The datasets were rigorously curated through pseudoalignment, sequence ID analysis, batch correction, and two-point normalization. Datasets were binned across three age groups: young (18-35 years old), middle-aged (35-65), and old (older than 65).

Our results show that a set of 300 genes is sufficient to predict an individual's muscle age with a mean absolute error of 8.6. Our study represents the first comprehensive effort to predict age based on muscle tissue gene expression profiles at this scale that can be used to predict the biological age of the muscle.

Our methodology extends existing approaches by effectively generalizing across diverse data sources, ensuring independence from project-specific biases and ethnicities, enhancing applicability in real-world scenarios.

The genes identified in our study hold potential implications for understanding the molecular basis of aging-related processes in muscle. Furthermore, these findings provide a foundation for future research to develop targeted interventions for sarcopenia. In ongoing work, we plan to integrate these genes into a microRNA regulatory network model to identify potential therapeutic targets for sarcopenia, underscoring the translational relevance of our findings.

Emanated from research conducted with the financial support of Science Foundation Ireland under Grant number [18/CRT/6214]



Abstract

Dual Delivery of Anti-Cancer Drugs using Metal-Organic Frameworks

Mc Hugh, K.1, Papatriantafyllopoulou, C.2

1 and 2. School of Biological and Chemical Sciences

Metal-Organic Frameworks (MOFs) have the potential to offset some of these side effects by being target specific, encapsulating the drugs until the tumour sites and then releasing the drugs. This is due to their high porosity, low cytotoxicity, good biocompatibility, and biodegradability. MOFs allow for a slower release of the drugs, preventing the burst effect caused by immediate release of the drug1. Although the potential of MOFs as drug carriers has been well established, their use in combinatorial treatments that involve more than one drugs has been less investigated. Dual drug delivery would improve the potency of the anti-cancer treatment because of the synergistic effect of the two drugs. Dual drug delivery can also help to overcome the multidrug resistance effect that comes from cancer cells becoming resistant to anti-cancer drugs. With the above in mind, we decided to explore the potential of MOFs as multiple drug carriers. For this purpose, NUIG4 was used. NUIG4 holds the record in doxorubicin (DOX) uptake, it is water stable and biocompatible, and protects the healthy cells from the drug cytotoxicity. Herein, the capacity of NUIG4 to deliver dox or mitoxantrone (MIT) and 5-fluorouracil (5-FU) is reported. Each anti-cancer drug that are used in this project have a different mechanism of action; this can help to overcome multidrug resistance. 5fluorouracil intercepts the replication of the cancer cells genetic material, due to the cancer cells mistaking 5-fluorouracil for uracil, while doxorubicin hydrochloride intercepts the replication process of the cancer cells by DNA intercalation, it slots itself between the base pairs of DNA. Mitoxantrone is a synthetic anti-cancer drug which is similar in structure to anthracycline drugs, such as doxorubicin hydrochloride. It has a similar mechanism of action to that of doxorubicin hydrochloride. The initial results suggest the successful encapsulation of DOX/ MIT and 5-FU, and a controlled release of the drugs, as a result of the large pore size and subsequent large internal surface area.



Fig. 1 Representation of the crystal structure of NUIG4.



Abstract

Identification of Potential Neoantigens in Cancer-Associated
Fibroblasts Isolated from Breast Cancer Patients
<u>Ryan, K.1,2</u> , O'Connor, D.3, Digby, B.1,2, Barkley, L.R.*3, Ó Broin, P.*1.
1. School of Mathematical & Statistical Sciences, University of Galway, Ireland
2. The SFI Centre for Research Training in Genomics Data Science, Ireland
3. Lambe Institute for Translational Research, University of Galway, Ireland
* These authors jointly directed this work

INTRODUCTION

Cancer-associated fibroblasts (CAFs) are a heterogeneous cell type found in the tumour microenvironment (TME). CAFs support tumour growth and metastasis and contribute to therapeutic resistance. They also impact immune infiltration and immune responses in the TME. Therefore, therapeutic targeting of CAFs is a viable strategy to treat cancer. Here, we aim to identify somatic mutations in CAFs, which may potentially give rise to neoantigens. Ultimately, we aim to elucidate the therapeutic potential of targeting CAFs by exploiting CAF-specific neoantigens.

MATERIALS AND METHODS

CAFs and corresponding tumour-associated normal fibroblasts (TANs) were cultured from tissue of 12 breast cancer patients (11 Luminal A and one triple-negative). Bulk RNA-sequencing was carried out on all samples. Leveraging reference datasets, CIBERSORTx [PMID:31960376] was used to characterise CAFs and TANs into fibroblast subpopulations. Whole-exome sequencing (WES) was carried out on CAFs and TANs from six patients. Landscape of Effective Neoantigens Software (LENS) was used to identify CAF-specific neoantigens [PMID:37184881].

RESULTS AND DISCUSSION

Our findings confirm the heterogeneity of our patient-derived CAFs and TANs, with the immunosuppressive-myofibroblastic subpopulation being predominant. This is important as pro-tumourigenic subpopulations must be identified to design effective CAF-targeting therapies. We also observed differences in the inferred proportion of CAF subpopulations, including antigen-presenting and vascular CAFs, between CAFs and TANs. WES identified 13 private missense mutations, with five of the six patients exhibiting one or more such variants. Interestingly, genes with these mutations included CAF markers and genes implicated in lipid metabolic pathways. CAFs contribute to lipid metabolism within the TME, thus impacting cancer progression and tumour immunogenicity.

In this study, we have identified candidate neoantigens in breast cancer CAFs. The next step is their validation using T-cell immunogenicity assays. These studies may help to unravel the potential of targeting CAF neoantigens to enhance the efficacy of anti-cancer therapy.



Abstract

The genetic contribution to variation in aortic distensibility	
<u>Chopra, m.c_{1,2}</u> Hynes, n.h _{3,4} , Seoighe, c.s _{1,2} .	
1. School of Mathematical & Statistical Sciences, University of Galway, Ireland	
2. The SFI Centre for Research Training in Genomics Data Science, Ireland	
3. Department of Vascular Surgery and Endovascular Surgery, Galway Clinic, Royal	
College of Surgeons in Ireland and University of Galway, Galway Affiliated Hospital,	
Doughiska, Ireland	
4. CORRIB-CURAM-Vascular Group, University of Galway, Galway, Ireland	

INTRODUCTION

Aortic distensibility is a risk factor underlying several cardiovascular events, however the contributing genetic factors remain unknown. This study aimed to understand the genetics of aortic distensibility utilizing genotypic and cardiovascular magnetic resonance images (CMRI) data from the UK Biobank (UKBB). Novel deconvolution methods have been explored to investigate the age-associated changes in the cellular composition of aortic samples obtained from GTEx. Furthermore, polygenic scores (PGS) will be calculated to determine whether they are associated with thoracic aortic aneurysm or dissection.

MATERIALS AND METHODS

To find the aortic distensibility, an existing deep learning convolutional neural network (CNN) was applied on 62,497 CMRI from the UKBB. Further, quality checks allowed us to exclude the CMRI which may affect the segmentation accuracy and measurement of distensibility. Following quality checks, GWAS was carried out on the aortic distensibility of 56,765 participants. To examine the cellular mechanism and age-related shifts in cellular proportions, we utilized CIBERSORTx deconvolution on aortic gene expression data from 432 GTEx participants. In the future, we intend to calculate PGS on GTEx genotypic samples generated from the loci associated with distensibility. We also plan to compute PGS on the remaining UKB samples to see if they are linked to thoracic aortic aneurysm or dissection.

RESULTS AND DISCUSSION

Aortic distensibility is a direct measure of aortic stiffness that can be accurately obtained from CMRI. The CNN network enabled us to calculate the distensibility for 56,765 subjects from CMRI. Furthermore, a two-stage GWAS on distensibility helped us grasp the significance of incorporating variables in the research to minimize erroneous positives. The deconvolution method helped us identify changes in the cellular composition of aorta associated with ageing. Furthermore, the PGS calculated from loci associated with distensibility will help us explain the link of this important physiological phenotype to aortic disease risk.



Abstract

COMPARATIVE ASSESSMENT OF COPY NUMBER ALTERATION CALLING TOOLS FOR THE IDENTIFICATION OF MALIGNANT CELLS IN AN ACUTE MYELOID LEUKAEMIA SINGLE-CELL RNA SEQUENCING DATASET

<u>Ó Dálaigh, M.</u>^{1,2,3}, Ennis, S. ^{1,2,3}, Conforte, A. ³, Washington, L. ⁴, Coughlan, S. ^{1,2}, Ó Broin, P. ^{1,2}, Szegezdi, E. ^{1,3}

 ¹SFI Centre for Research Training in Genomics Data Science
 ²School of Mathematical and Statistical Sciences
 ³Apoptosis Research Centre, School of Biological and Chemical Sciences
 ⁴Biological Engineering, Data Driven Biology, National Science Foundation Research Traineeship, University of California, Santa Barbra, United States of America

INTRODUCTION

Acute myeloid leukaemia (AML) is an aggressive malignancy, resulting in the accumulation of poorly differentiated white blood cells in the bone marrow (BM). In AML, normal and malignant haematopoiesis take place simultaneously. The malignant cells share features with normal haematopoietic cells which makes identifying the malignant cells a challenging task.

Single cell transcriptomics (scRNA-seq) data have been used in recent years to infer the presence of copy number alterations (CNAs) which are a feature of cancer cells. We hypothesised that AML cells may differ from normal haematopoietic cells in this regard which could enable us to separate these cell populations.

METHODS

We previously performed scRNA-seq on 28 longitudinal samples (diagnosis, remission, relapse) from BM aspirates of 10 AML patients. In this project we evaluated the ability of three CNA profiling tools (inferCNV, CopyKAT, Numbat) to identify the leukaemic cells based on altered CNA profiles. InferCNV and CopyKAT use expression levels of adjacent genes to infer genomic copy numbers, while Numbat integrates additional allelic ratio and haplotype data to identify CNAs present.

RESULTS

CopyKAT and Numbat differed in their malignant predictions (41% overlap) with the concordance of these predictions showing variability between individual samples. InferCNV does not provide malignant predictions. In an effort to extract these annotations, we first tested for the presence of multiple clusters (tumour vs normal) in the inferCNV-generated data with methods proposed for scRNA-seq data. Only 1 sample had evidence of multiple clusters. Clustering these cells into 2 clusters with hierarchical clustering generated annotations more similar to CopyKAT than to Numbat.

CONCLUSION

Numbat was deemed to be the most promising tool due to its ability to produce malignant cell labels as well as to identify loss of heterozygosity CNA events which would be invisible to CopyKAT and Numbat which rely solely on gene expression.



College of Science and Engineering, Research and Innovation Day 2024 Abstract

Evaluating Foundational AI Against Traditional Machine Learning	
Models in Early Stage Lung Cancer Relapse Prediction	

<u>Timilsina, Mohan₁</u>, Curry, Edward₁

1. Data Science Institute, Insight Centre for Data Analytics

ABSTRACT

We assessed foundational AI and large language models (LLMs) for predicting non-small-cell lung cancer (NSCLC) relapse, using data from 1,348 patients. Our study juxtaposes traditional machine learning methods with LLMs like Mistral-7B and Random Forest. Results show Random Forest's slight edge in precision-recall, but Mistral-7B excels in identifying rare relapse events, crucial for early detection and improving patient care.

INTRODUCTION

The potential of Foundation Models for predicting lung cancer relapse using tabular data is significant but not yet fully realized. These models, particularly those with cross-table transferability, require task-specific fine-tuning, unlike the more seamless applications in language and vision. The current need for fine-tuning underscores a challenge in their direct use for lung cancer prognosis.

MATERIALS AND METHODS

- The dataset is utilized from Spanish Lung Cancer Group (EU-Horizon Project)
- A workflow serializes tabular data into text for lung cancer relapse prediction.
- Classical algorithms are optimized and validated for performance.
- An LLM is refined and improved using predictive outcomes.

RESULTS AND DISCUSSION

- Random Forest performs slightly higher than Mistral-7B in AUC-PR for relapse prediction task.
- Both models effectively identify the minority relapse class in imbalanced dataset.
- Random Forest leads in overall metrics.
- The close AUC-PR scores of Random Forest and Mistral-7B are particularly relevant for clinical diagnostics.



Fig: 1 Solution approach to our relapse prediction pipeline

Туре	Models	AUC-PR	AUC-ROC	Accuracy
	QDA	0.377 ± 0.009	0.525 ± 0.016	0.415 ± 0.024
	SVC	0.438 ± 0.089	0.538 ± 0.108	0.636 ± 0.001
	KNeighbors	0.449 ± 0.042	0.580 ± 0.045	0.621 ± 0.022
	Decision Tree	0.455 ± 0.019	0.632 ± 0.018	0.659 ± 0.022
	Label Propagation	0.456 ± 0.040	0.579 ± 0.052	0.634 ± 0.033
	Label Spreading	0.483 ± 0.046	0.580 ± 0.053	0.636 ± 0.037
Supervised Classification	Gaussian NB	0.517 ± 0.022	0.671 ± 0.014	0.628 ± 0.065
	MLP Classifier	0.635 ± 0.010	0.745 ± 0.018	0.694 ± 0.021
	LDA	0.670 ± 0.046	0.758 ± 0.025	0.715 ± 0.029
	AdaBoost	0.683 ± 0.088	0.760 ± 0.061	0.729 ± 0.041
	Logistic Regression	0.687 ± 0.044	0.771 ± 0.026	0.717 ± 0.031
	Gradient Boosting	0.710 ± 0.080	0.778 ± 0.058	0.732 ± 0.048
	Random Forest	0.719 ± 0.080	0.787 ± 0.058	0.746 ± 0.043
	DistilBERT	0.385	0.513	0.364
Zero-Shot Classification	RoBERTa	0.394	0.502	0.556
	BART	0.375	0.50	0.549
	GPT-2	0.654	0.621	0.575
Fine-Tuning Classification	GPT-NEO-125M	0.661	0.663	0.631
	BERT	0.661	0.651	0.632
	Falcon-7B	0.686	0.672	0.625
	LLaMA-7B	0.681	0.680	0.615
	Mistral-7B	0.701	0.671	0.605
Polotivo Impre	vement	2.56%	15 73%	18.03%

Table: 1 Results from classical ML and the LLM models



Abstract

Osteoporotic Mineral Crystallinity and Estrogen-Deficiency alter Mineralization in a 3D Mineralized		
Bone Model		
Khabooshani, MKH ¹ , Naqvi, SMN ¹ , Von Euw, SVE ² , McNamara, LM ¹		
1. Mechanobiology and Medical Devices Research Group (MMDRG), University of		
Galway School,		
2. School of Biological and Chemical Sciences, University of Galway, Ireland		

INTRODUCTION

Our in vitro studies have demonstrated that the mechanobiological responses of osteoblasts and osteocytes can be impaired during estrogen deficiency. However, changes in bone crystallinity arise during osteoporosis, but how these changes influence osteocyte differentiation and mineralization are not yet fully understood. Here we build upon previous studies by developing models that are highly mineralised with different crystallinities to mimic the composition of mature bone tissue and study osteoporosis.

MATERIALS AND METHODS

Novel bone-like proxies were prepared using platelet-shaped carbonated hydroxyapatite nanoparticles (nHA) coated with different proportions of hydrated amorphous surface layer (HASL), at compositions representing healthy (HE: 35%) and osteoporotic (OS: 20%) bone mineral. These proxies were incorporated with gelatin (8% wt.) at varying relative concentrations (50%, 25%, or 12.5% w/w). Osteoblasts (MC3T3-E1) were pre-treated with 17β-Estradiol for 4 days and then encapsulated within the gelatin-nHA hydrogels (10^6 cells/ml). Over 21 days, these hydrogels were cultured with17β-Estradiol (E) or without estrogen (EW). TEM, XRD, SSNMR, biochemical assays (DNA, ALP, and calcium content), histological staining (DMP1/actin, Von-Kossa), mechanical testing, and micro-CT scanning were conducted to assess osteogenic differentiation and mineralization.

RESULTS AND DISCUSSION

MC3T3-E1 cells formed dendritic cell processes by day 21 (Fig 4A), indicating cellular differentiation. DNA analysis indicated reduction in cell number in 12.5% nHA on day 21 (Fig 4C), possibly due to reduced proliferation during differentiation. DMP1 staining confirmed osteocyte differentiation, with higher intensity in 12.5% nHA in OS (Fig 4G). ALP activity decreased in EW groups (Fig 4D). Calcium deposition was higher in OS groups under both E and EW conditions, especially in the 12.5% nHA groups (Fig 4E). Von-Kossa and micro-CT analysis confirmed mineral deposition, with more deposition under estrogen withdrawal, particularly in OS groups under estrogen withdrawal, particularly of 12.5% nHA (Fig 4F, H). Compression stiffness was higher in osteoporotic (OS) groups under estrogen withdrawal, particularly for 12.5% nHA (Fig 4B). We propose that new mineral deposition_is higher for osteoporotic proxies due to changes in nHA surface water content and synergistic effects of estrogen deficiency on mineral content.



Abstract

Advancements and Applications of Generative Artificial Intelligence in Medical Imaging
<u>Farooq, Muhammad Ali₁, Abaid, Aymen₂, Yao, Wang₁, Ullah, Ihsan₂ , Corcoran, Peter₁</u>
1. School of Engineering, C3I Group, University of Galway
2. School of Computer Science, University of Galway

ABSTRACT

Generative artificial intelligence (AI) has emerged as a transformative technology in medical imaging, revolutionizing the field by generating realistic and high-quality images with potential applications in diagnosis, treatment planning, and medical research. This work explores the recent advancements and diverse applications of generative AI techniques in medical imaging. Keeping this in view we have investigated the potential usage of large stable diffusion models as a viable solution to render high quality novel synthetic data for two different medical imaging applications which includes synthesizing dermoscopic images (1. diffusion based Dermoscopic imaging: DbDI) for malignant skin cancer diagnosis and rendering synthetic cardiac CTA (2. diffusion CTA: dCTA) images for Type B Aortic Dissection (TBAD). This is achieved by fine-tuning text to image diffusion model by employing few shot learning methodology to cut the requirements for large training sets and further save the computational cost as well. The synthesized data serves multiple purposes, serving as both a novel training set to augment diversity within training data and as a comprehensive test set to assess the robustness and efficacy of fine-tuned deep learning models through cross-validation.

INTRODUCTION

Few-shot learning, a subfield of machine learning, offers a promising approach for leveraging Stable Diffusion to render medical imaging data. Few-shot learning techniques aim to train machine learning models with only a small number of examples, making them ideal for scenarios where large datasets are unavailable or impractical to obtain. By harnessing the capabilities of few-shot learning in conjunction with Stable Diffusion, it becomes possible to generate synthetic medical imaging data that closely resembles real-world images, thereby expanding the availability of training data for downstream tasks such as image segmentation, classification, and disease diagnosis.

MATERIALS AND METHODS

1. Data Processing Pipeline



Figure 1: Image preprocessing pipeline for removing clutters and further resizing the image to 512x512 resolution.



Coláiste na hEolaíochta & na hInnealtóireachta College of Science & Engineering

College of Science and Engineering, Inaugural Research and Innovation Day 2024

Effects of Estrogen Deficiency on 3D Vascularized and Humanized Bone Model under Mechanical Stimulation

Bukhari, MMM¹, Naqvi, SM¹ and McNamara, LM¹

¹Mechanobiology and Medical Device Research Group, Biomedical Engineering, School of Engineering

INTRODUCTION

Osteoporosis causes fundamental changes in bone composition and bone cell responses to mechanical loads. We recently developed a simplified 3D model of bone to provide an insight into the mechanisms governing these changes, and uncovered the effect of estrogen deficiency on mineralization and mechanosensitivity of osteocytes. This research seeks to build upon these studies, particularly by providing advanced mineralisation bone models that are mimic bone tissue *in vivo*. Vascularisation can promote mineralization *in vitro* and *in vivo*, particularly during endochondral ossification. Thus, here we followed an endochondral ossification priming approach to develop a 3D vascularized bone model to study estrogen deficiency and bone mineralization under mechanical stimulation.

MATERIALS AND METHODS

Human bone marrow stem cells (HBMSCs) (P5) were encapsulated in gelatin-mtgase (3% V/V) and cultured with growth factors to develop a chondrogenic template. At day 22 (endothelial cells) HUVECs, osteoblasts and HBMSCs were added to the chondrogenic template to initiate vascularization. Constructs were cultured in osteogenic media with estrogen supplementation until day 43. Estrogen was withdrawn from the constructs at day 43 and then these were cultured for a further 21 days (until day 63). Mechanical stimulation was applied for 21 days (from day 43 to day 63) by compression in a bioreactor (MechanoCulture TX). Biochemical assays, histological staining and real time PCR analysed the effects of vascularization and estrogen deficiency on mineralization.

RESULTS AND DISCUSSION

The current study provides an *in vitro* 3D vascularized and humanized bone model that recapitulates estrogen deficiency representative of the osteoporotic bone phenotype. During endochondral ossification the vasculature infiltrates the lacunae and release chemokines to attract osteogenic cells and initiate bone formation. We confirmed the presence of CD31+ distinct vessel-like structures (Fig. 1B) and report that estrogen deficiency reduces vascularization (Fig. 1C). There was a significant increase in mineralization and matrix formation in the vascularized and estrogen withdrawal group, at day 63 (Fig. 1 E, K, G, M). Estrogen deficiency decreases the number blood vessels and fatty acid metabolism, leading to increased number of adipocytes and decreased bone mineral (1). Here we also report a reduced endothelial cells numbers, whereas in our vascular model estrogen deficiency leads to an increase in the mineral deposition. This contradiction might be due to differential responses of human and mouse cells in the presence of vascular cells under estrogen deficiency. Our ongoing studies are exploring the molecular interactions between vascular cells and osteoblasts during estrogen deficiency and mechanical stimulation.



Figure 1: (A) Alcian blue staining of chondrogenic template. (B, C) CD31(green), Actin (red), DAPI (blue) immunofluorescence staining, yellow arrows indicate multicellular vessel. (D) Fluorescence intensity of CD31. (E) Von kossa staining at day 63, green arrows indicate mineral nodules. (F, G, L, M) Immunohistochemistry for Collagen I and X at day 63. (H, I, J) Gene expression for DMP-1, OPN and RANKL/OPG normalized to NV-E+. (K) Calcium content normalized to DNA. Significant differences (p < 0.05) indicated relative to E (*) and NV (#).

1. Rodrigues, Julia, et al J Cardiovasc. Dis. Res. 2019



Abstract

Machine Learning Enhanced Impedance Probe For Real-time Monitoring Of Perfusion In Free Flaps Post Micro-reconstructive Surgeries In The Head And Neck Region

Meselmanil, N.¹, Biggs, M. *¹ ¹ CÚRAM, University of Galway, Ireland.

Micro-reconstructive surgery of the head and neck regions utilize a autograft termed a "free flap" to repair anatomical and aesthetic defects¹. These flaps can fail due to postoperative vascular perfusion complications resulting in tissue ischemia and transplant failure, increasing patient morbidity^{2,3}. Conventional postoperative monitoring relies on intermittent and subjective assessment via a clinician who monitors the graft colour and temperature, an approach which is frequently insufficient for the detection of early on-set ischemia^{4,5}. This issue **highlights the need for improved monitoring methods** that provide real-time data for timely corrective intervention within the first 48 hours post-surgery^{3,6}, when most complications manifest.

This study introduces an innovative monitoring approach **leveraging electrical impedance spectroscopy (EIS) integrated with machine learning**. By measuring the electrical properties of tissues, EIS can detect subtle perfusion changes^{7,8}, offering timely and reliable feedback on the perfusion status of the flap post-surgery. This system aims to improve patient outcomes by enabling clinicians to identify and address compromised perfusion before irreversible damage occurs.

Materials and Methods:

A pilot system employing a Solartron Analytical Materials Lab XM impedance analyzer, and a geometrically optimized microneedle electrode array (Figure 2) was designed. The machine learning model was developed in Python. Integration with LabView, aimed at automating both data acquisition and prediction is planned. To simulate tissue states, cucumbers served as phantoms allowing for the distinction of normal versus a low perfusion (dehydrated) state. Features extracted from the impedance data included modulus, phase angle, and both real and imaginary components of impedance at each frequency. It is planned to develop a portable prototype and benchmark it against the results of the pilot system. Once validated, testing on human tissues is intended to train the machine learning model for assessing perfusion. The performance of Random Forest, Support Vector Machine (SVM), and a simple Neural Network was evaluated using accuracy metrics and confusion matrices.

Results and Discussion:

Impedance modulus and Phase measurements showed clear differentiation between fresh and dehydrated cucumbers, representing normal-perfusion and low-perfusion tissue respectively (Figure 3A). Subsequent machine learning analysis identified significant variations between the hydrated and dehydrated states with 99% accuracy, indicating the system's capability to detect changes in perfusion similar to those in human tissue. The neural network model, in particular, showed high performance with zero false negatives and only one false positive out of the entire test set.

Conclusion:

These results underscore the potential of EIS coupled with machine learning to provide a robust and sensitive means of monitoring tissue health in real-time.



Abstract

ADVANCEMENTS IN PH SENSOR DESIGN FOR CONTINUOUS AND MINIMALLY INVASIVE ASPHYXIA MONITORING

Hussain, N.M.^{1,2,*}, Kraśny, M.J.^{2,3}, Amin, B.^{1,2,3}, O'Halloran, M.^{1,2,3}, and Elahi, A.^{1,2}

- 1. Electrical and Electronic Engineering, University of Galway, H91 TK33, Galway, Ireland
- 2. Translational Medical Device Lab, University of Galway, H91 TK33, Galway, Ireland
- 3. School of Medicine, University of Galway, H91 TK33, Galway, Ireland

INTRODUCTION

Arterial blood gas (ABG) analysis is commonly used for diagnosing asphyxia (a condition arising when the body is deprived of oxygen), but its invasive and intermittent nature poses challenges, especially in neonates. Interstitial fluid (ISF) offers a more sensitive alternative for detecting asphyxia and metabolic disorders due to its limited buffering capacity, however, raises several technology challenges. To address limitations of accessing ISF for biosensor development, in our previous study we developed and characterized ISF-mimicking solutions to mimic the pH and electrical properties of ISF. This study aimed investigation of alternative pH measuring methods to facilitate design of a real-time biosensing applications required for asphyxia monitoring.

MATERIALS AND METHODS

ISF-mimicking buffer solutions, including sodium phosphate (SP), BES, and bis-tris propane (BTP) buffers, were prepared at 0.1M concentration at room temperature using deionized water. ITO-glass slides were used to fabricate sensing electrodes compatible with electrochemical impedance spectroscopy (EIS) technology. The frequency-dependent complex impedance data were acquired using Metrohm Autolab PGSTAT204 potentiostat. In this study we investigated the EIS method within the frequency range from 10 Hz to 100 kHz, various buffer configurations and temperature dependency.

RESULTS AND DISCUSSION

The study results indicate that the configuration of ITO-electrodes and the mode of operation in EIS measurements significantly influences the accuracy for pH and impedance measurements. Through comprehensive analysis across various temperatures, probe configurations, and PGSTAT204 modes of operation, this study has led to a preference for the three-electrode potentiostat probe setup at measured temperatures due to its reduced impedance and consistent output, which is crucial for the development of highly sensitive and precise pH biosensors. The findings of this study have laid a foundational basis for future research to advance the design and functionality of EIS based sensors, with the goal of improving their sensitivity, accuracy, and suitability necessary for biosensor development in real-time asphyxia monitoring.



Abstract

Effect of extracellular vesicles derived from licensed and unlicensed MSCs on B cell function and
activation
Kallens, P. C. ¹ , Williams, M. ² , Malinova, D. ² , Brennan, M ¹
¹ University of Galway, Galway, Ireland, ² Queen's University Belfast, Belfast, United Kingdom

Autoimmune diseases (ADs) are characterized by B cell function dysregulation. Novel therapies have significant side effects. Mesenchymal stem cells (MSCs) have been proposed as an alternative therapy for ADs, due to their potent immunomodulatory capacities, particularly when exposed to inflammatory conditions ('licensing'). MSCs-derived extracellular vesicles (EVs) have been proposed as safer alternative to MSCs. The aim of this study was to evaluate the effect of EVs derived from licensed and unlicensed MSCs on B cell function and activation.

Bone marrow murine MSCs (BM-MSCs) were cultured on tissue culture plastic until 70% confluency. Cells were then incubated in EV-depleted media with IFN- γ and TNF- α to 'license' them, or in standard conditions, for 48 hours. The conditioned media was then collected, and the MSCs-EVs were isolated by size exclusion chromatography. EVs samples' particle and protein concentrations were measured by NTA and BCA, respectively.

B cells were isolated from an allogeneic strain mouse and activated in vitro. The effect of licensed and unlicensed EVs on the expression of surface markers and proliferation of B cells was measured by flow cytometry.

'Licensed' EVs could modulate the expression activation markers MHCII, CD80, CD69 and CD86 on activated allogeneic murine B cells. EVs were also capable of modulating B cell proliferation.

Our findings demonstrate that BM-MSCs-derived EVs can modulate B cell activation and function *in vitro*. Moreover, our study highlights the influence of MSCs' culture conditions on EV effects, suggesting potential therapeutic versatility in diseases characterized by immune dysregulation. Further elucidation of the mechanisms is crucial to fully harness the clinical potential of MSCs-derived EVs.



Abstract

A $S_{180}F$ mutation in D-alanine aminotransferase increases resistance to β -chloro-D-alanine in Staphylococcus aureus

Roy, Rakesh and O'Gara, James P.

Microbiology, School of Biological and Chemical Sciences, University of Galway, Ireland

INTRODUCTION: D-alanine (D-ala) is a critical amino acid essential for synthesis of the bacterial cell wall, which is the target of beta-lactam and other antibiotics. Key enzymatic reactions responsible for synthesis of D-ala include alanine racemase (Alr), which converts L-alanine to D-alanine and D-alanine aminotransferase (Dat), which converts pyruvate to D-alanine in a reaction dependent on D-glutamate. We previously reported that impaired alanine transport heightens the susceptibility of methicillin-resistant *Staphylococcus aureus* (MRSA) to the β -lactam antibiotic oxacillin (OX) and D-cycloserine (DCS), an alanine analogue drug that inhibits Alr. Furthermore, OX and DCS act synergistically which has therapeutic potential in the treatment of MRSA infections. To further investigate the therapeutic potential of targeting D-ala biosynthesis, we used directed evolution to generate a mutant resistant to β -chloro-D-alanine (BCDA), another alanine analogue drug reported to target Alr and D-alanine aminotransferase (Dat).

RESULTS AND DISCUSSION: Genome sequencing revealed a single point mutation in *dat*, resulting in a predicted $S_{180}F$ substitution in the BCDA1 mutant strain. The *dat* gene is part of a 2-gene operon downstream of the *pepV* dipeptidase gene. Expression of the *pepV-dat*_{S180F} operon significantly increased BCDA resistance in wild-type MRSA, whereas wild-type *pepV-dat* had no effect. Experiments to compare the enzymatic activity of recombinant Dat and Dat_{S180F} are underway. Protein structure modeling followed by superimposition analysis suggests that the S_{180F} substitution alters the conformation of the protein. Bioinformatic docking binding analysis revealed a higher affinity of BCDA for Dat_{S180F}. Protein-Ligand Interaction Profiler analysis further indicated that additional bonds are formed between BCDA and Dat_{S180F}. Our working hypothesis is that the higher affinity of Dat_{S180F} for BCDA protects Alr from inhibition by this antibiotic suggesting that combinations of BCDA and DCS to ensure inhibition of both Alr and Dat may have significant therapeutic potential against MRSA.



Abstract

Pursuit of Digital Innovation in Psychiatric Data Handling Practices in Irish Mental Health Services
Zeeshan, R. 1
¹ College of Science and Engineering

Ireland is ranked among the most disadvantageous European countries in terms of mental health challenges. This study's objective was to examine the state of data handling practices in the Irish Mental Health Services (MHS), identify the shortcomings regarding privacy, security, and usability of psychiatric case notes, and propose an innovative technological solution which addresses most of the surfaced challenges. We evaluated the standard psychiatric record management protocols being followed in Irish MHS as a case study using extensive mixed methodology that involved a thorough literature-review, ethical approval, online surveys with mental-health professionals as participants, interviews of psychiatrists, interactions with mental-health organizations, analysis of inspection reports by the Ireland Mental Health Commission (MHC), and comparative evaluation of existing IT solutions.

Our study revealed outdated data-management, heavy reliance on paperwork resulting in serious repercussions, parallel workload, alarmingly low readability of notes, and a non-viable setup that hinders research and analytical examination. Our survey reported an average score of 4.37/10 given by participants in terms of technology utilization. Regarding privacy measures, 75 percent of participants mentioned that staff members are allowed to keep their phones while accessing psychiatric case notes. Similarly, 80 percent submissions highlighted that multiple staff members can access sensitive notes and patients' contact information. On the other hand, MHC reports showed that their inspections are limited to evaluating physical privacy only. Regarding technological comparative analysis, we observed that conventional IT solutions are vulnerable against cyberattacks and fall short in addressing multiple challenges simultaneously. Therefore, an innovative convergence of different technologies is needed. Our research supports speech-to-text transcription for data collection, interactive AI for data analysis, and permissioned blockchain for data storage and retrieval. Our survey participants also estimated the proposed solution to optimize their workload by an average of 35 percent.

Irish MHS seem to be handling psychiatric data under polycrisis circumstances, and therefore a single dimensional digitization of records would not be sufficient in addressing the wide range of concerns. In addition to highlighting intertwined challenges in Irish Psychiatry and validating the need for innovation in data handling practices in Irish MHS, this study culminated in the proposal of an innovative technological solution that offers a significant contribution to a considerably improved, efficient and compliant service delivery in mental healthcare.



Abstract

A STATISTICAL MECHANICS INVESTIGATION OF DYNAMIC SARCOMERE AND TITIN ORGANISATION IN CARDIAC MYOCYTES

Coleman, R.J., McGarry, P.

Department of Biomedical Engineering, University of Galway

INTRODUCTION

Culture methods for human induced pluripotent stem cell cardiac myocytes (HiPSC-CMs) rely on ad hoc applied mechanical stimuli to induce cell maturation and sarcomere formation [1]. We propose a thermodynamically based model to predict the formation of sarcomeres.

METHODS

Our thermodynamic framework to model growth of sarcomeres predicts remodelling within CMs of the three state system of actin-myosin, consisting of unbound cytoskeletal proteins \hat{N}_U , stress fibres \hat{N}_{BF} , and sarcomeres \hat{N}_S . Remodelling is predicted by converging to thermodynamic equilibrium in actin-myosin species, where remodelling of sarcomeres from SFs is expressed

$$\frac{\partial \widehat{N}_{S|F}}{\partial t}\omega_{S|F}^{-1} = G_{S|F}\left(\widehat{N}_U + \widehat{N}_{BF}\right)\exp\left(\widehat{n}_S\frac{\mu_B(\theta) - \mu_{ZF}}{k_BT}\right) - M_{S|F}\widehat{N}_S\exp\left(\widehat{n}_S\frac{\mu_H - \mu_{ZF}}{k_BT}\right).$$
(1)

Enthalpy of sarcomeres μ_H is composed of contributions from ground state enthalpy, strain energy, work associated with cross-bridge binding, and an energetic contribution of titin.

RESULTS AND DISCUSSION

Our thermodynamic framework accurately predicts the key experimental observation of increasing sarcomere formation under cyclic loading of increasing applied strain magnitude (Fig.1A). A corresponding computed increase in contractile stress due to increased sarcomere/myofibril formation is also strongly aligned with experimental measurements (Fig1.B). The computed contribution of sarcomeres, stress fibres, titin, and passive cell components to contractile stress during a loading cycle is shown in Fig.1C.



Figure 1: HiPSC-CMs under 1 Hz biaxial loading. A) Evolution of sarcomere concentration. B) Contractile stress after 10 days loading, alongside experimental values [3]. C) Contractile stress in final loading cycle.

Our thermodynamic framework strongly aligns with observations of increasing active contractility and sarcomere evolution [2]. This theoretical modelling framework has the potential to predict organ-level remodelling and provide a new understanding of the biomechanical conditions leading to the onset and progression of cardiac hypertrophy [4].

References & Acknowledgements

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Abstract

Advancing Cancer Diagnosis and Prognosis through Integrated Liquid Biopsy Data Management:	
The CLuB Initiative	
Hooshmand, S. A. <u>.1</u>	
1 School Of Mathematics, Statistic & Applied Mathematics	

Current research interests

My research focuses on the integration and management of liquid biopsy data for improved cancer diagnosis and prognosis. As part of the Cancer Liquid Biopsies Consortium (CLuB), I am streamlining the processing and storage of clinical and genomic data from breast, ovarian, lung, and pancreatic cancers. This involves extending and deploying the cBioPortal web application on AWS for improved accessibility and functionality for the liquid biopsy research community, while ensuring data security with frameworks like Keycloak, and developing user-friendly web tools for seamless data management. Once our datahas been integrated with public datasets, we will employ advanced computational methods such as machine learning, deep learning, and network analysis to helps uncover novel insights into cancer biology. Through these endeavors, CLuB accelerates diagnostic innovation and professional training in cancer research.

Research activities

Grants :

This research was supported by the North-South Research Programme administered by the Higher Education Authority on behalf of the Department of Further and Higher Education, Research, Innovation and Science and the Shared Island Fund (CLuB: The All-Ireland Cancer Liquid Biopsies Consortium <u>https://www.clubcancer.ie</u>).

Conferences :

Irish Computational Biology and Genomics Symposium, December 2023, Galway; All-Ireland Cancer Liquid Biopsies Consortium (CLuB) Symposium, October 2023, Dublin

Memberships:

EACR



Abstract

Multi-omic integration of <u>c</u> ancer <u>l</u> iq <u>u</u> id <u>b</u> iopsy data: An All-Ireland approach
<u>Hooshmand, Seyed Aghil₁, Ó Broin</u>
<u>, Pilib₂.</u>
1. School of Mathematics, Statistics and Applied Mathematics, National University of
Ireland, Galway, Ireland
2. School of Mathematics, Statistics and Applied Mathematics, National University of
Ireland, Galway, Ireland

My research focuses on the integration and management of liquid biopsy data for improved cancer diagnosis and prognosis. As part of the Cancer Liquid Biopsies Consortium (CLuB), I am streamlining the processing and storage of clinical and genomic data from breast, ovarian, lung, and pancreatic cancers. This involves extending and deploying the cBioPortal web application on AWS for improved accessibility and functionality for the liquid biopsy research community, while ensuring data security with frameworks like Keycloak, and developing user-friendly web tools for seamless data management. Once our datahas been integrated with public datasets, we will employ advanced computational methods such as machine learning, deep learning, and network analysis to helps uncover novel insights into cancer biology. Through these endeavors, CLuB accelerates diagnostic innovation and professional training in cancer research.

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Abstract

A 40-amino acid amphipathic helix in the C-terminal of *Fasciola hepatica* helminth defense molecule (FhHDM-C2) alters macrophage lysosomal pH, regulates pro-inflammatory responses, and exhibits potent biotherapeutic activity in murine Experimental Autoimmune Encephalomyelitis

Lalor, R.¹, Tanaka, A.², Shiels J.³, Dixit, A⁴, Hoadley, S.⁴, Dufourd, E.⁴, Hamon, S.¹, To, J.² Taggart, C.C.³, Weldon, S.³, O'Brien, B.², Greer, J.⁴, Dalton, J.P.¹, <u>Donnelly, S.¹²</u>

¹Molecular Parasitology Laboratory, Centre of One Health (COH) and Ryan Institute, School of Natural Science, University of Galway, Ireland.

²School of Life Sciences, University of Technology Sydney, Ultimo, Sydney, Australia. ³ Wellcome-Wolfson Institute for Experimental Medicine, Queen's University Belfast, Northern Ireland.

⁴The University of Queensland, UQ Centre for Clinical Research, Brisbane, Queensland, Australia

INTRODUCTION

The Helminth Defense Molecules (HDM) are a family of immune regulatory peptides exclusively expressed by trematode worms. The 68 amino acid HDM secreted by the liver fluke *Fasciola hepatica*, FhHDM-1, is the archetypal member of this family and considered essential to the success of this global parasite of humans and livestock. We have previously demonstrated that *in vivo* FhHDM-1 regulated macrophage responses to inflammation-inducing ligands, thereby ameliorating the progression of immune-mediated tissue damage in several murine models of inflammatory disease.

MATERIALS AND METHODS

We postulated that an understanding of the structure-function relationship of the HDMs would facilitate the design of highly efficacious biotherapeutic peptides. Using a combination of bioinformatics, structural analyses, and cellular assays we have now identified the minimal bioactive peptide (40 amino acids) derivative of FhHDM-1 that regulates macrophage activation by inflammatory ligands.

RESULTS AND DISCUSSION

This peptide derivative, termed FhHDM-1.C2, contains a five amino acid motif at its N-terminus, which facilitates cellular interaction and uptake, and an amphipathic a-helix within the C-terminus, which is necessary for lysosomal vATPase inhibitory activity, with both regions linked by a short unstructured segment. As a readily synthesisable FhHDM-1.C2 peptide exhibits enhanced regulation of macrophage function, as compared to the full-length FhHDM-1, and potent prevention of the progression of relapsing-remitting-experimental autoimmune encephalomyelitis (EAE) when administered therapeutically following the onset of first paralysis. The protective effect of FhHDM-1.C2 is not associated with global immune suppression, which places the HDM peptides as a new, improved class of therapeutics for the treatment of multiple inflammatory diseases. Comparative analyses of the HDMs from various major zoonotic trematodes revealed a similar capacity for immune regulation. Further, sequence variations of their C2 derivatives point to parasite-specific mechanisms of immune regulation, possibly related to their tissue location. These important new advances into the structure-function relationship of the lead HDM peptide, FhHDM-1, encourages further prospecting and screening of the broader trematode family of peptides for the discovery of novel and potent immune-biotherapeutics.


Abstract

Difference between bipolar patients and healthy participants across the structure-function coupling gradient

Lastname1, a.b₁, Lastname2, c.d₂.

<u>Dahan, s₁₃₄, Ó Broin,p₂, Cannon, m.d_{3,4}</u>

- 1. The SFI Centre for Research Training in Genomics Data Science, Ireland
- 2. School of Mathematical & Statistical Sciences, University of Galway, Ireland,
- 3. Center for Neuroimaging Cognition and Genomics, University of Galway, Galway, Ireland
- 4. Clinical Neuroimaging Laboratory, Galway Neuroscience Centre, College of Medicine Nursing and Health Sciences, University of Galway, Galway, Ireland

INTRODUCTION

Structural MRI studies suggest differences in Bipolar disorder (BD) patients compared to controls. Findings from fMRI studies show aberrant connectivity in known resting-state networks in BD patients. Recent studies look at coupling of structural connectivity (i.e., physical connections between regions) and functional connectivity (i.e., statistical dependency in activation between regions). This coupling reflects the relationship between structural connections and functional connections. Structure-function coupling was found to differ in BD patients, although results from different studies point to different coupling strengths and involved regions. Coupling was found to vary between brain region across a gradient, whereby unimodal regions have strong coupling, and transmodal regions, have weaker coupling. This study aims to look at regional differences in coupling between BD patients and controls.

MATERIALS AND METHODS

The study includes 162 controls and 163 BD patients from the UK Biobank. Functional regionbased connectivity matrices were calculated from the time series of 554 brain parcels, obtained from the Schaefer atlas and the Melbourne Atlas. The same parcellation was used to obtain structural connectivity matrices. For each region, multilinear regression was performed with structural connectivity properties of all edges for a given region as the predictors and the functional edges connecting the region to all other regions were predicted. Then the R² scores were calculated between the observed and the predicted functional connectivity. Then a T-test for each region was conducted between the BD group and controls.

RESULTS AND DISCUSSION

After multiple testing Bonferroni correction, one region showed a significant difference in the regional coupling between BD group and controls. The significant region is in the prefrontal cortex and is involved in the executive control network, which has been linked to BD in previous studies. The findings of this study agree with previous findings that relate connectivity of the executive control network to BD.



Abstract

BIOINFORMATICS REFINEMENT OF CRISPR-CAS9 KNOCKOUT SCREENS ANALYSIS UNCOVERS ERRATIC SGRNAS AND ADDITIONAL GENES MODULATING CELL RESPONSES TO CDC7 INHIBITORS

Bernard, S^{1,2}, Rainey, M.D², Ryan, C.J^{1,3}, Santocanale, C^{1,2}

¹SFI Centre for Research Training in Genomics Data Science

²Centre for Chromosome Biology, School of Biological and Chemical Sciences, University of Galway, Ireland

³UCD Cancer Data Lab, Conway Institute of Biomolecular and Biomedical Research, School of Computer Science, University College Dublin, Ireland

The Cell Division Cycle 7 (CDC7) kinase promotes DNA synthesis by activating the origins of replication. CDC7 is highly expressed in cancers, which led to the development of CDC7 inhibitors (CDC7is) as anti-cancer drugs. The anti-proliferative activity of CDC7is greatly varies in different cell lines possibly because of cell-type specific gene function.

To identify genes determining the cell sensitivity to CDC7is, we performed a genome-wide CRISPR-Cas9 screen in MCF10A cells. Cas9 uses a sgRNA to target a gene causing loss of function mutations in most situations. Typically, CRISPR screens are performed with multiple sgRNAs targeting each protein-coding gene. Our library was composed of ~150,000 sgRNAs targeting ~19,000 protein-coding genes with 8 sgRNAs per gene. We identified both genes that sensitize and promote resistance to CDC7is. Interestingly, we detected 7,478 sgRNAs behaving differently from the others that target the same gene (erratic sgRNAs). The phenotype induced by these erratic sgRNAs may derived from off-target effects, or a mutation at specific regions of the targeted gene affecting a protein domain and a subset of protein functions.

To deconvolute this complexity, we constructed a bioinformatics pipeline to filter all sgRNAs targeting multiple locations and suspected for off-target activity, thus generating a sub-library containing ontarget sgRNA. Reanalysis of the CRISPR screen was performed using the refined sgRNA library uncovering additional genes that might regulate cell responses to CDC7is, which were missed in the earlier analysis. We then built a second pipeline to properly annotate all sgRNAs by using UniProt and ENSEMBL functional annotation data, and output every information into a single PDF file. This pipeline can help the identification of proteins that, if altered in certain functional domains, have biological relevance to the cellular responses to CDC7is. Both pipelines can be further developed to help all researchers performing CRISPR-Cas9 screen analysis.



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College of Science and Engineering, Research and Innovation Day 2024

Changes in mechanical properties contribute to breast cancer stemness with matrix stiffness and mechanical stimulation resulting in reduced spheroid number and increased stemness markers.

Senthilkumar¹, S., Mofehintioluwa¹, A., and Naqvi¹, S.M. ¹ School of Engineering (Biomedical), College of Science & Engineering, University of Galway

INTRODUCTION: Understanding the mechanisms that govern cancer metastasis is vital for developing effective strategies to combat the disease. Previous studies have explored the effects of stiffness on cancer cell behaviour^{(1-2).} For example, increased matrix stiffness has been shown to directly activate Epithelial- Mesenchymal Transition (EMT), tumour invasion, and metastasis through the EMT-inducing transcription factor TWIST1⁽¹⁾. However, in addition to changes in stiffness, hydrostatic pressure in the tumour interstitium is also considerably increased in breast cancer^(3,4). The current study seeks to advance our understanding of how hydrostatic pressure may drive cancer cells to transition from a proliferative to a metastatic state. Our specific objective is to investigate the specific roles of matrix stiffness and hydrostatic pressure in influencing the stemness properties of 4T1 breast cancer cells.

MATERIALS AND METHODS: 4T1 cell encapsulated gelatin was enzymatically crosslinked with varying concentrations of microbial transglutaminase to create hydrogels with different stiffnesses (1.7 kPa and 4.5 kPa). These hydrogels were then placed in gas-permeable, water-impermeable EVO Cell Culture bags, and maintained at 37°C. The bags were divided into two groups: (1) static and (2) mechanically stimulated. For mechanical stimulation, intermittent hydrostatic pressure of 53 mmHg (mimetic of breast cancer⁽⁵⁾) was applied to the hydrogels daily for 1 hour over 7 days. We assessed the hydrogels at day 7 to examine Cell Proliferation and Spheroid Size (Ki67, H&E), evaluate Epithelial-Mesenchymal Transition (EMT) (E-Cadherin, N-Cadherin) and Stemness (NANOG, OCT4, SOX2).

RESULTS AND DISCUSSION: Under mechanical stimulation cancer cell proliferation and spheroid number and size was lower compared to static conditions in soft hydrogels suggesting that hydrostatic pressure may influence transition of cancer cells from a proliferative profile to a metastatic profile⁽⁶⁾. Reduced cell proliferation is associated with a migratory phenotype, regulated by Y-box binding protein 1 (YB-1)⁽⁶⁾, which is also linked to EMT-inducing transcription factor TWIST1⁽⁷⁾. The reduction in E-cadherin staining under mechanical stimulation suggests that hydrostatic pressure can weaken cell adhesion, potentially facilitating cancer cell movement and metastasis by reducing cell adhesion and tissue integrity⁽⁸⁾. The increase in N-cadherin expression under mechanical stimulation in soft hydrogels suggests that the hydrostatic pressure may promote cancer metastasis by facilitating cancer cell migration and invasion through changes in adhesion properties⁽⁹⁾. The increased expression of stemness proteins OCT4, NANOG and SOX2 under mechanical stimulation in soft hydrogels suggests that the hydrostatic pressure induces cancer stemness.



Figure 1: Ki67 staining (A) and intensity (B); H&E staining (yellow arrows indicate spheroids) (C). Cell area measured using Image J (D); E-Cadherin staining (E) and Intensity (F); N-Cadherin staining (G) and Intensity (H); OCT4 Intensity, (I) SOX2 Intensity (J), and NANOG Intensity (K).

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Abstract

The Lectin Pathway of Complement Regulation by the infectious *Fasciola hepatica* newly excysted juvenile (NEJs)

Kilbane, T.¹, Dobó, J.², Gál, P.², Cwiklinski, K.³, Dalton, J. P.¹, De Marco Verissimo, C.¹ ¹ Molecular Parasitology Laboratory, Centre for One Health and Ryan Institute. University of Galway, Ireland.

² Institute of Enzymology, Research Centre for Natural Sciences, Budapest, Hungary. ³ Institute of Infection, Veterinary and Ecological Sciences, University of Liverpool, UK.

The complement response is the first-line innate host defence against invading organisms and is activated via Classical, Lectin, and Alternative pathways. The Lectin pathway (LP) initiates with recognition molecules binding to sugar arrays on pathogen surfaces, leading to C3-convertase formation and propagation of the cascade. Recently, we showed that the invasive stage of *Fasciola hepatica*, newly excysted juveniles (NEJs), survives in normal human serum by inactivating the complement LP, despite being covered by glycans. In the present study, we observed that neither of the main LP recognition molecules, Mannosebinding lectin (MBL) and Ficolin-2 (Fic-2), bind to live NEJs. We discovered that 1h of incubation at 37°C of rhMBL or rhFic-2 with either live NEJs or their excreted-secreted (ES) molecules alone results in rhMBL/rhFic-2 specific cleavage. Considering the collagen-like domains in MBL and Fic-2 and the well-established collagenolytic activity of the cathepsin L3 protease (FhCL3), secreted by NEJs, we next co-incubated these molecules at 37°C showing that rFhCL3 efficiently cleaves rhMBL and rhFic-2. Fascinatingly, our studies show that F. hepatica NEJs possess multiple strategies to prevent LP activation, which also include the expression and secretion of serine protease inhibitors (Serpins; FhSrp1 and FhSrp2). We demonstrate that rFhSrp1 and rFhSrp2 inhibit the MBL-associated serine proteases (MASP-1 and MASP-2), the key initiators of the LP. These inhibitors form complexes and inhibit rMASP-1/2, as shown by ELISAs, SDS-Page, biochemical assays, and Mass spectrometry (MS). Furthermore, rFhSrp1 or rFhSrp2 alone are able to selectively inhibit the LP (>90%).

The downstream effect of MASPs inhibition was verified by a proportional reduction in their ability to cleave complement C4, essential for forming C3-convertase. Here, we uncovered an array of novel mechanisms by which the invading life-stage of *F. hepatica* become refractory to killing via the host LP, emphasizing the importance of complement regulation by this parasite.



Abstract

Osteogenic factors alter the effects of estrogen withdrawal in post-menopausal osteoporotic
models: A long-term in vitro study
<u>O' Brien, T.M</u> ¹ , Naqvi S.M ¹ , and McNamara, L.M ¹
¹ Mechanobiology and Medical Device Research Group, Biomedical Engineering, University of
Galway.

INTRODUCTION: Bone tissue composition becomes more heterogeneous in an osteoporotic animal model and estrogen deficiency alters osteoblast and osteocyte activity [1-5]. However, these studies were conducted for short durations. Osteogenic factors (dexamethasone, L-ascorbate, β -glycerophosphate) are commonly used in vitro to induce osteoblastogenesis and enhance mineralisation [6]. However, the interaction between osteogenic factors and estrogen withdrawal on osteoblast and osteocyte activity is unknown. Therefore, the objectives are to (1) establish a multicellular model of postmenopausal osteoporosis in long-term culture to attain highly mineralised, mechanically representative constructs of mature bone, and (2) investigate the influence of osteogenic factors (OF) on mineralisation, paracrine signalling and osteogenic differentiation.

METHODS: Osteocytes (OCY454) and osteoblasts (MC3T3-E1) were pre-treated with 17 β -Estradiol and encapsulated in gelatin-nHa-mtgase hydrogels for 85 days, as follows: (1) E OF+: continued estrogen with OF, (2) E OF-: estrogen without OF, (3) EW OF+: estrogen withdrawal with OF, and (4) EW OF-: estrogen withdrawal without OF. Osteoclast precursors (RAW264.7) were added and allowed to differentiate for 14 days. ALP assays and OPG ELISAs were conducted to determine osteogenic activity and paracrine signalling. Mineralisation was measured by micro-CT scanning (μ CT100, Scanco), calcium assays and by EDX (XFlash 6/60, Bruker). Cellular morphology was visualised using SEM (Hitachi, S2600) and H+E staining.

RESULTS AND DISCUSSION: Osteogenic groups had significantly higher calcium concentration (D69, D98), calcium (D98), phosphorus (%) and BV/TV(%) relative to groups without OF (Fig.1A, 1D, 1E, 1F, 1G). ALP activity was initially elevated in all groups but declined by D98 (Fig.1H). Mineralisation was detectable only at D98 by micro-CT in groups without OF (zoom boxes, Fig.1C). Osteoclasts were confirmed by SEM and H+E staining (Fig.1B). This study provides a novel understanding of the mitigating effects of osteogenic factors in estrogen withdrawal models for osteoporotic research, suggesting their role in modulating osteoblast and osteocyte responses.

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Abstract

Elucidating the structure-function relationship and mechanism of xylooligosaccharides as commensal probiotics

<u>Umapathy, U. 1</u>, Villegas-Moreno, J. 1, Joshi, L. 1, Kilcoyne, M. 1 University of Galway

Xylan and xylooligosaccharides (XOS) from wood are proposed as next-generation probiotics for improving the intestinal microbiome for human and animal health. However, it is still unclear whether xylan or XOS are more beneficial for gut bacteria, what mechanism is utilised by bacteria to degrade xylan and XOS, and whether XOS preferences and utilisation mechanisms are different in human and bovine digestive systems. This study examined the utilisation of xylan and XOS by four gut-associated Lactobacillus species; two human-associated (Lacticaseibacillus rhamnosus, Lacticaseibacillus paracasei) and two human- and bovine-associated (Lactobacillus acidophilus, Lactobacillus brevis). Bacterial growth was monitored for 16 h in media supplemented with different concentrations of xylan, XOS (lengths 1-6), or an XOS mixture. Supernatants were analysed for XOSs using HPLC analysis. Xylosidase and xylanase activity over time in supernatant and cell lysate was monitored by colourimetric assay. Prebiotic properties of some Lactobacillus strains were increased up to 14% with xylan and 64% with XOS. While xylan was utilised by all species, XOS of different lengths were preferred by different species and some lengths were growth inhibitory at certain concentrations. Xylanase was produced after 24 h in the presence of xylan, while xylosidase was produced within 2 h for all Lactobacillus species. Overall, the beneficial properties of xylan and XOS depend on the concentration of prebiotic supplements, length of XOS and Lactobacillus strain (human or bovine-associated) and time of enzyme production. This work could lead to formulations specifically targeting human or bovine gut health.



Abstract

Quality monitoring during embedded bioprinting
using integrated microscopy and computer vision.
Sergis, V. ^{1,4} , Kelly, D. ^{1,4} , Pramanick, A. ¹ , Mason, K. ³ , Daly, A. ^{1,2,*} .
¹ CÚRAM, SFI Research Centre for Medical Devices, National University of Ireland
Galway, Galway, Ireland
² Biomedical Engineering, National University of Ireland Galway, Galway, Ireland
³ School of Computer Science, University of Galway, University Road, Galway, Ireland
⁴ Equal contribution

INTRODUCTION

Granular hydrogels are increasingly employed as support materials due to their shear-thinning and self-healing properties that are essential for the embedded bioprinting process. Despite widespread use, determining general design criteria is yet unaddressed, including optimal particle morphology and size. Herein, agarose support hydrogels are developed with varied particle morphologies to explore their influence on rheological behaviour and printing quality.

METHODS

A novel inline microscope camera setup is utilized to capture the embedded bioprinting process, while image processing and classical computer vision techniques are employed for data analysis. Four metrics are defined to evaluate print quality: percentage of overlapping area between the physical and CAD model, percentage of area covered by excess extruded ink, average printed structure width, and average error distance of the printed structure's centreline from the desired print path.

RESULTS AND DISCUSSION

Thixotropic behaviour and instantaneous recovery to the initial point emerge as crucial factors. Interestingly, lower viscosity support hydrogels with irregular particle morphologies exhibit improved extrusion consistency, likely due to enhanced particle-particle interactions. The integration of the novel microscope camera setup and computer vision analysis not only provides comprehensive insights into embedded bioprinting processes and particle-particle interactions in granular support hydrogels but also pioneers a novel approach in bioprinting technology, aiming in enhanced print fidelity.



Figure 1: The embedded bioprinting process (a), the camera field of view in two different support bath solutions (b), and the subsequent analysis of results (c).



Ollscoil NA Gaillimhe University of Galway

Coláiste na hEolaíochta & na hInnealtoireachta College of Science & Engineering

SUSTAINABLE FUTURES





Abstract

Revealing the impact of biomass mechanism on the performance of anaerobic system
Abdolvahed Noori, Guangxue Wu*
Civil Engineering, School of Engineering, College of Science and Engineering, University
of Galway, Galway, H91 TK33, Ireland

INTRODUCTION

Sulphate-laden wastewater originated from industrial and human activities have become a potential threat to the environmental security. Anaerobic digestion (AD) is promising for treating high-strength wastewater. On the other hand, environmental protection and increasing demand for renewable energy have resulted in the development of anaerobic digestion and biogas production [Ren et al. 2018]. The biological approach utilizing sulphate-reducing bacteria (SRB) in the AD system to treat sulphate containing wastewater has gained broad attention. AD is an efficient system that can be employed to not only remove sulphate but also recover resources such as biofuel from waste, remediate waste/water, and reduce greenhouse gas emissions.

MATERIALS AND METHODS

Four anaerobic reactors (5L, $35 \pm 1 \circ C$), two sequencing batch reactors (SBR), and two continuous flow reactors (CFR), with solids retention times (SRT) of 15 days and 30 days were employed under rapidand slow-filling modes with substrate ethanol as the main organic carbon source. The four ethanol-fed reactors, named as SBR15, SBR30, CFR15, and CFR30 fed with COD to SO_4^{2-} ratio 5:1. The organic loading rate (OLR) and the sulphate concentration in the influent were 4 kg COD/(m₃·d) and 800 mg/L. Other components in the synthetic wastewater included nutrients and trace element fed into the reactor were referred to [Du et al. 2021]. During the long-term operation, sulphate reduction, methane production rate continuously was analysed.

RESULTS AND DISCUSSION

Based on long-term operation, rapid-feeding mode SBR15 and SBR30 exhibited higher methane production (418.5 ml/L) and (489.5 ml/L) respectively than slow-feeding mode CFR15 and CFR30 (318.9 ml/L) and (356.8 ml/L) respectively (Fig 1). Total suspended solid (TSS) concentration reached to 1.26 g/L, 1.35 g/L, 1.11 g/L, 1.21 g/L for SBR15, SBR30, CFR15, and CFR30 respectively (Table 1). Furthermore, all reactors exhibited 99% sulphate reduction with COD removal of over 90%.

Acknowledgements

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CFR CFR SBR SBR Reactor (SRT5) (SRT30) (SRT15) (SRT30) 1.26 SS (g/L) 1.11 1.21 1.35 ${\rm SO_4}^{2-}$ 99% 99% 99% 99% reduction Table 1. Total suspend solid (TSS) concentration and sulphate reduction percentage



Abstract

ENVISIONING NET-ZERO: MULTI-STAKEHOLDER STRATEGIES FOR DECARBONIZATION ZONES IN IRELAND

Alexandrov, A. a.b1, Goggins, J.c.d2

- 1. PhD Researcher, CONNECTED, Construct Innovate Research Center, School of Engineering, College of Science & Engineering, University of Galway
- 2. Established Professor of Civil Engineering, Director of Construct Innovate; Co-Principal Investigator in MaREI Centre, Ryan Institute; Academic Manager, ERBE Centre for Doctoral Training, School of Engineering, College of Science & Engineering, University of Galway

INTRODUCTION

This study explores the collaborative design of decarbonization zones in Ireland as a strategy to meet the 2030 and 2050 Climate Action goals. It focuses on fostering multi-stakeholder engagement for sustainable futures and innovative solution development, aiming to ensure that Ireland's decarbonization efforts are not only technically feasible but also socially equitable and collaboratively supported.

MATERIALS AND METHODS

This research employs an inter-disciplinary approach integrating qualitative and collaborative methodologies to explore the formation and operation of decarbonization zones in Ireland. Delphi interviews with climate action officers form the primary qualitative method, providing structured, expert-driven insights that guide the co-design process. These interviews are used for assessing the current landscape of local climate action initiatives and for identifying barriers and resources in climate collaboration.

Additionally, the study draws insights from engaging with a diverse group of stakeholders, including local government officials, community leaders, and academic experts. These engagements are facilitated through the Connected project's co-design framework, which utilizes 'climate action community tools' to map out essential resources, effectively engage stakeholders, and bridge climate knowledge gaps.

RESULTS Preliminary insights reveal significant barriers to effective collaboration in implementing decarbonization zones, including a lack of cohesive vision and an imagination crisis. To counter these, the study proposes developing future scenarios through multi-stakeholder workshops, leveraging the co-design framework to envision sustainable net-zero emission environments. These scenarios aim to bridge current capabilities with future needs, fostering innovation and community empowerment in climate action.

The co-creation of **future scenarios** addresses the imagination crisis by proposing diverse, practical solutions developed through inclusive, community-focused approaches.

The intended **poster will illustrate this exploratory journey**, showcasing the early stages of moving

AND

DISCUSSION



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from conceptual frameworks to actionable, community-supported strategies for climate action.

Keywords: *climate action, future scenarios, multi-stakeholders, sustainable development, imagination crisis, decarbonization zones, collaborative design, inter-disciplinarity, action research.*



Abstract

Sustainable Futures: Lead the transition to a sustainable future through innovation solution development
Eftekhari, A., 1
¹ The University of Galway, Ireland
As the global community confronts the escalating challenges of climate change, Ireland stands at the forefront of pioneering sustainable solutions. With a significant portion of its population living near the coast and a substantial marine territory that exceeds its land area, Ireland's environmental and economic stability is intrinsically linked to the health of its marine environments. This paper integrates findings from multiple studies assessing the impacts of climate change on Ireland's marine ecosystems and outlining innovative strategies for their sustainable management.



Abstract

Card Payment Protocol for Cryptocurrencies with Payment Channel Network
De Silva, A. 1, Thakur, S. 2, Breslin, J. 3
1, Data Science Institute
¹ , Data Science Institute Cryptocurrency, despite its recent surge as a speculative investment, has yet to become a widely accepted means of exchange. The complexity of the technology presents a significant obstacle for the general public in adopting it as a payment medium. Thus, simplifying the payment process is a crucial necessity. Facilitating the adoption of conventional payment instruments, for example, can bring convenience to both merchants and consumers. In this work, we propose a novel cryptocurrency card payment protocol that leverages the Payment Channel Network (PCN) concept, providing high throughput and affordable transactions. Our design is based on the Bitcoin-backed Lightning Network (LN) with adjustments to make it executable by a smart card. It preserves the decentralized nature of cryptocurrencies, reduces operational costs, and allows for instant settlement of payments as compared to both conventional and cryptocurrency card payment systems. Our game theoretical analysis models the engagement between the cardholder and the card agent as a long-run extensive form game. The results show that they comply with the protocol without suffering any honest loss under pragmatic conditions. Additionally, we discuss the privacy features of our protocol compared to conventional card payments and LN. The protocol can operate independently, without the need for trust, and can also be regulated for those seeking government mediation. Our proposed approach has the potential to revolutionize the payment landscape by allowing the public to use cryptocurrency for everyday transactions conveniently and enabling existing cryptocurrency holders to conduct affordable micropayments while preserving the decentralized and secure nature of cryptocurrencies.



Abstract

Prediction of Strain Values on Wind Turbine Blade Incorporating Artificial Intelligence Tool

Ahmad, A.₁, Jiang, Y.₁, Finnegan, W.₁, Goggins, J.₁

1. Construct Innovate and SFI MaREI Research Centre, Ryan Institute, School of Engineering, University of Galway, H91 TK33, Galway, Ireland

INTRODUCTION

Physical testing is an essential way of assuring the structural integrity, effectiveness, and security of a wind turbine blade. Structural testing a blade is a direct way to identify potential flaws, examine the performance criteria, and optimize design attributes. However, testing wind turbine blades is also considered a challenging task because it is time and cost consuming. Therefore, the application of artificial intelligence (AI) tools, such as gene expression programming, random forest, decision tree, bagging, and Adaboost approaches, are of great interest to researchers. These tools have the capability by using the test data to train the model which can give the predicted outcome in a limited time period.

MATERIALS AND METHODS

This study uses an AI bagging model to predict strain values at different locations of the wind turbine blade. The data set was collected from the static testing of the 13-meter-long wind turbine blade. The bagging model was run on the test data using Python coding in Anaconda Navigator (Spyder) software. The model was trained using 70% of the data set, while the remaining 30% was used for testing. The 10-fold cross-validation method was employed to validate the bagging model. The metrics such as coefficient of determination (R²) were used to evaluate the precision of the model. During the validation process, the mean absolute error (MAE) and root mean square error (RMSE) were also to confirm the model's legitimacy in predicting strain values on the wind turbine blade.

RESULTS AND DISCUSSION

The bagging model shows an accurate and precise relationship between the experimental results of the wind turbine blade and the predicted outcome, giving the R^2 value equal to 0.999 as depicted in the Figure 1(a). However, the difference between the experimental and predicted strain results (Errors value) is shown in Figure 1(b). Moreover, the 10-fold cross-validation confirms the bagging model's precision level by indicating lower error values and a high R^2 (0.999) value during the process. The values of MAE and RMSE during the 10-fold process were reported as 3.94µm and 7.86µm, respectively. The application of AI tools for investigating the behaviour of blade material under different loading conditions would provide valuable insights for enhancing blade design and performance optimization.





Abstract

Investigating the Impacts of Energy Renovation Strategies on Indoor Environmental Quality: the ENABLE Project
<u>Wijeyesekera, W.B₁</u> , Byrne, M ₁ , O'Donnell,J ₂ , Agahamolaei,R ₄ J. McGrath ₃
 School of Natural Sciences, Centre for Climate Change and Air Pollution studies (C- CAPS), University of Galway
2. School of Mechanical and Materials Engineering, University College Dublin (UCD)
3. Department of Experimental Physics, ICARUS Climate Research Centre, Maynooth
University

4. School of Mechanical and Manufacturing Engineering, Dublin City University

INTRODUCTION

As concern grows about the impact of climate change, the need for more sustainable energy technologies is highlighted, as adapting of such technologies will have a major impact both on the environment and on human populations. The built environment sector consumes a significant amount of energy, and building regulations across the globe are being modified in order to adopt a more sustainable and a greener model. In this, it is important that both the operational and embodied energy needs of buildings are considered in greener building design, and residential buildings merit particular consideration. In that context, it is imperative to consider the potential harmful impacts that may arise through introducing new energy strategies especially within domestic residential buildings, and these impacts include indoor air quality which, if compromised, may have adverse health effects on building occupants.

This presentation will describe the key objectives of the ENABLE project, one aspect of which is the development of a novel knowledge-based library that can be used as a decision-making tool in designing energy efficient residential buildings with appropriate indoor environmental quality for Ireland. The project will focus on 500,000 Irish domestic dwellings and will consider the optimum cost trade-off between the building's whole life-cycle energy performance analysis and the required indoor environmental quality metrics.

MATERIALS AND METHODS

Computational simulations for pre and post retrofit scenarios will be completed. This is to understand and compare the behaviour of different air pollutants for pre and post retrofit case scenarios.



Abstract

MARKET DRIVEN MATERIALS SELECTION FOR THERMOPLASTIC FLEXIBLE RISER PIPELINES USED IN OFFSHORE AND SUBSEA APPLICATIONS

C.I. Bachour^{1,2,3*}, R.M. O'Higgins², N.M. Harrison^{1,2,3}, R. Allen³, T. Flanagan³

¹ Mechanical Engineering, College of Engineering & Informatics, University of Galway, Ireland
 ² School of Engineering and Bernal Institute, University of Limerick, Ireland
 ³ Éire Composites Teo, An Choill Rua, H91Y923 Indreabhán, Ireland.

INTRODUCTION

The most economic oil & gas transportation method rely on pipelines [1]. In the case of submarine pipelines, different types (design, materials) of pipelines can be used depending on the operating depth and the type of product transported, as illustrated in Fig.1 – A. Composite materials have emerged as a competitive lightweight piping option for off-shore Carbon Capture and Storage (CCS) applications such as Enhanced Oil Recovery, where CO_2 is injected to help oil extraction. CCS consists in capturing CO_2 mainly from Oil & Gas cleaning processes, and transporting it towards secure geologic sites, such as depleted sub-sea oil or gas fields [1]. This project involves material selection for the development of global scale flexible Thermoplastic Composite Pipeline (TCP) compatible with CCS technologies manufactured by a scalable cylindrical method, such as Automated Tape Placement (ATP). The TCP consists of three bonded layers i.e. polymer liner, intermediate composite laminate (responsible for pipe's structural integrity) and polymer cover (see Fig.1 – B). Benchmark materials selection was based on commercially available TP systems.

MATERIALS AND METHODS

Using the GRANTA selector software [2], material indices (MIs) were used to assess the performance of the intermediate laminate manufactured by ATP (see Fig.1 - B). After several Trade-off plots were developed, 36 record were filtered from a pull out of 4,192 available records.

RESULTS AND DISCUSSION

Although the reinforcement with the greatest potential were found to be PP matrix are steel, basalt and asbestos continuous fibers, due to cost and provider availability PP/CF was chosen as the final option based on cost benefit analysis. Prototyping of the pipe assembly and subsequent mechanical testing are expected to confirm structural integrity of the light-weight pipe.

FIGURES



Fig. 1: (A) General picture of the different types of submarine flexible pipelines that can be used in offshore applications. (B) Schematic of flexible risers. Layers are bonded to each other. Up - Lateral view [3] and down – elevation view [4].



Abstract

Investigating the impact of the Trombe wall on indoor thermal comfort using CFD

Sirin, C.1.2, Goggins, J.1,2,3, Hajdukiewicz, M.1,2,3

¹School of Engineering, College of Science and Engineering, University of Galway, Galway, Ireland

²MaREI Research Centre for Energy, Climate and Marine, and Ryan Institute, University of Galway,

Galway, Ireland

³Construct Innovate, University of Galway, Galway, Ireland

INTRODUCTION

The adoption of passive solutions for heating and cooling has become a key point in the effort to achieve low-energy buildings. Maximising the use of renewable energy systems and contributing to the reduction of heating and cooling energy demand are one of the main goals of net-zero energy buildings. Sustainable design and green construction practices are effective solutions to provide comfortable thermal conditions for occupants while decreasing the seasonal heating demand in buildings. TWs help to prevent overheating-overcooling problems in buildings.

MATERIALS AND METHODS

Trombe walls (TWs) are building components that can be used to regulate indoor thermal environment. Utilising TWs as a passive heating and cooling method, can help in providing desirable indoor comfort conditions while reducing the reliance on the mechanical systems. This study investigates different types of TWs and their impact on the indoor environment. The results of this numerical study show the impact of utilising different TW materials on indoor thermal conditions. Moreover, the indoor temperature stratification and airflow patterns are carefully explored and evaluated against the indoor comfort criteria.

The study simulates indoor conditions in a typical dwelling room using computational fluid dynamics (CFD). The CFD analysis allows to investigate the effectiveness of integrating different types of TWs within residential buildings to improve their performance.

RESULTS AND DISCUSSION

According to the results, the type of material used directly affects the thermal performance of the Trombe wall.



Abstract

A Toolkit for Uplifting Green Public Procurement in Irish Public Sector for Sustainable Future.
<u>Anagipura D.J.P.D.₁, Carragher V.₁, Goggins J.₁</u>
1. College of Science & Engineering. School of Engineering. University of Galway. Ireland.

INTRODUCTION

Green Public Procurement (GPP) is a crucial driver for a sustainable future. However, lack of resources and the knowledge gaps often hinders its effective implementation. The research project (named GAPS) addresses this challenge by developing a comprehensive toolkit specifically for the Irish public sector. In this abstract it mainly considers on the findings from the recent survey conducted with experts in GPP to get their insights on barriers, drivers, and policy recommendations in GPP.

METHODOLOGY

GAPS employs a multi-faceted approach to develop its toolkit. Extensive desktop reviews, stakeholder consultations, and analysis of existing GPP best practices lay the foundation for informed decision-making. Case studies from diverse sectors were categorised under 22 themes to make it more accessible. Best practice is currently being identified through desktop review and participatory research with experts involved in state-of-the-art GPP policy and practice both in Ireland and Europe. Experts' insights were collected by conducting a survey and used discourse-based analysis (DBA) method in performing the survey (see Fig 1). These findings will disseminate through the toolkit for the stakeholder to make informed about GPP.



Figure 1: Geographical diversity of the participants.

IMPACT

The GAPS toolkit will empower Irish public bodies to make informed decisions when procuring goods, services, and infrastructure, ensuring that their procurement choices align with environmental and sustainability goals. This will foster a shift towards greener procurement



practices, and it pave the path for a sustainable future.

CONCLUSION

In conclusion, the GAPS project, enriched by insights from discourse-based analysis with GPP experts, represents a pivotal step towards a greener, more sustainable future for Ireland. By addressing the complexities of GPP comprehensively, our toolkit serves as a roadmap for navigating the intricate landscape of sustainable procurement. By addressing barriers, harnessing drivers, and implementing targeted policy interventions, stakeholders can unlock the full potential of GPP to drive positive environmental, social, and economic outcomes.



Abstract

Comparative analysis of the immune responses elicited by native versus recombinant *Fasciola hepatica* vaccines

López Corrales, J.¹, Lalor, R.¹, McEvoy, A.², Jewhurst, H.¹, Dorey, A. L.¹, De Marco Verissimo, C.¹, Keane, O. M.³, Cwiklinski, K.⁴, Dalton, J. P.¹

1. Molecular Parasitology Laboratory, University of Galway, Galway, Ireland.

- Animal & Bioscience Department, Teagasc Mellows Campus, Athenry, Co. Galway, Ireland.
 Animal & Bioscience Department, Teagasc Grange, Dunsany, Co. Meath, Ireland.
 - 4. Institute of Infection, Veterinary and Ecological Sciences, University of Liverpool, UK

INTRODUCTION

Fasciola hepatica or " common liver fluke" is one of the most prevalent helminths to negatively impact livestock globally. At present, anthelmintic drugs are the most commonly used control measure against fluke; however, the rapid rise in anthelmintic resistance to these chemicals has demonstrated that there is an urgent need for the development of alternative control therapies.

Vaccination is one approach currently being investigated as an alternative to drug use, as it has already been successfully used to eradicate many other infectious diseases in humans and animals. However, while vaccination using native and recombinant fluke antigens have yielded varying success in small animal studies, the same level of protection has not been observed in economically relevant ruminants.

MATERIALS AND METHODS

In this study, we report a vaccine strategy aimed at identifying combinations of fluke antigens from the excretory/secretory (E/S) products of adult fluke that can confer protection in sheep.

To identify candidate antigen cocktails, *F.hepatica* E/S was fractionated by size exclusion chromatography (SEC).

Proteomic analysis by MS was used to reveal the composition of each fraction, which was replicated recombinantly with the most abundant proteins of each fraction.

Sheep were immunised with native fractions or recombinant cocktails and subsequently experimentally infected with *Fasciola hepatica* metacercaria or naturally acquired infection on pasture.

Vaccine efficacy was determined by measuring cellular proliferation and antibody responses to antigens, parasitic burden, fecundity and animal weight gain.

CONCLUSION

- SEC separated *Fasciola hepatica* E/S into 4 distinct fractions.
- Vaccination with native fractions elicited strong cell mediated responses to fluke antigen similar to their recombinant counterparts, however antibody responses differed dependant on antigen.
- A recombinant vaccine cocktail composed of glycolytic enzymes reduced weight loss in sheep associated with experimental and naturally acquired fluke challenge.
- These studies highlight the positive impact vaccination can have on animal welfare parameters without statistically reducing parasite burden or fecundity.



Abstract

CFD analysis to estimate the hydrodynamic loadings on a horizontal axis tidal turbine during operation
<u>Xu, K_{1.2.3}</u> , Finnegan, W _{1,2,3} , Goggins, J _{1,2,3} , O'Rourke, F ₄ .
1. School of Engineering, University of Galway
2. Construct Innovate and the SFI MaREI Research Centre, Ryan Institute, University of
Galway
3. Dundalk Institute of Technology

INTRODUCTION

Tidal energy has attracted increasing attention in recent years, due to its vast potential and advantage over other renewables in terms of reliability. Horizontal axis tidal turbines are similar to wind turbines in geometry but experience a much higher loading due to the extreme conditions in the submarine environment. Consequently, the loadings on the tidal turbine need to be accurately evaluated within the design stage to ensure its long-term durability.

MATERIALS AND METHODS

In this research, a three-dimensional computational fluid dynamics (CFD) model of a horizontal axis tidal turbine rotor has been developed and validated by using the blade geometry of the prototype turbine used in the H2020 MaRINET2 Round Robin Tests. To study fluctuations of hydrodynamic loads on turbine blades, a numerical wave tank model is developed with calibrated wave parameters from the physical wave tank at the University of Galway as the input wave profile. Hydrodynamic experimental testing of 3D-printed scaled turbine models will be used for model validation, to investigate the fluid-structure interaction of the turbine in the presence of waves.

RESULTS AND DISCUSSION

The numerical results reveal that with increasing rotating speed of the tidal turbine, the thrust force that the turbine experiences increases, while the torque experiences a rise firstly, reaching a maximum value and then decreasing gradually. The experimental and many existing studies show that the ocean tidal turbine experiences frequent and large-scale fluctuations of hydrodynamic loads during operation, which may lead to blade fatigue damage. Therefore, the next stage of this research is fatigue loading evaluation, by combining the developed numerical wave tank with the previously developed turbine model, to improve the present fatigue design and testing of tidal turbine blades. In the long run, this study will support the development of tidal energy, while helping society achieve Net-Zero emissions by 2050.



Abstract

Review of recent developments in novel steel connections including intermeshed steel connections
<u>Bhatti, K. A.</u>
1. University of Galway

Why hasn't the digitization in construction industry progressed with the same pace as in the automotive sector, despite so much advancement in manufacturing, robotics assembly, and artificial intelligence/machine learning (AI/ML). There has been very limited progress in steel connections since the introduction of welding technology for over a century. Hence, the primary objective of ARISE is to minimize bolting/welded connection, facilitate faster erection and reduce labour involvement with the help of newly proposed connection system i.e. Intermeshed Steel Connections (ISCs), it will help facilitate digitization and robotics involvement in construction industry. The focus of this research is on the computational modelling and experimental testing of braced frames with ISCs on column-column and beam-column joints considering different types of lateral and gravity loadings. The analytical models shall be developed on FEM software (ABAQUS) with improved contact performances and load distributions. The results of all these analytical models, shall be compared with the experimental results obtained from small- and full-scale testing in the structure labs of University of Galway, University of Texas at San Antonio, New York University and Queen's University Belfast.



Abstract

Assessment of future wind power over offshore regions of Ireland using downscaled CMIP6.
<u>Rajagopal, a.b₁, Nash, c.d₁, Nolan, e.f₂</u>
 Department of Civil Engineering, College of Science & Engineering, University of Ireland Irish Centre for High-End Computing (ICHEC), Ireland

The study investigated the impacts of climate change on future Irish wind power using the latest downscaled CMIP6 (4km resolution). We assessed the impact of climate change on Ireland's offshore wind power by analysing high-resolution data from an ensemble of Regional Climate Model (RCM) simulations focused on offshore regions of Ireland. The four Shared Socioeconomic Pathway (SSP) scenarios (SSP126, SSP245, SSP370, and SSP585) were examined to study the projected future offshore wind power generation in Ireland.

To validate the downscaled CMIP6 data, various validation techniques were employed, including comparison with observational data from Met Eireann weather observing stations. Additionally, spatial data were validated using high-resolution WRF ERA-5 (2km) data for the period 1981–2010. Subsequently, analyses were conducted using future projections of wind speed by analysing the frequency of occurrence, Weibull distribution, coefficient of variation of mean wind power density, etc. Three future time periods—2021–2050, 2041–2070, and 2071-2100—were considered to investigate projected percentage changes in offshore wind power for all four SSP scenarios relative to the historical period 1981–2010. Additionally, dedicated analyses were conducted for areas designated for future offshore wind turbine projects, underscoring the significance of this research.

The results indicate a projected decrease in mean wind power density by the end of the century, particularly under the SSP5-8.5 scenario. Statistical analyses, utilizing the latest offshore turbine power curves, provide insights for manufacturers to effectively modify turbine efficiency and identify locations with higher wind power yield. These findings are crucial for optimizing the design and placement of offshore wind turbines, contributing to the sustainable development of wind energy resources in Ireland.



Abstract

How	Blockchain will disrupt and drive innovation in the Blue Economy
	<u>Santos, M1</u> , Breslin, J1.
1.	University of Galway, Unit for Social Semantics, Data Science Institute

The anthropogenic climate change is interfering with the stability and resilience of the Earth system and disrupting its life support systems, stressing the environment, the world economy, and societies worldwide. Ireland must, therefore, strive to adopt structural and transformative approaches, such as addressing Blue Economy challenges, for a climate resilient future, climate and food security, and prosperity.

Blue Economy refers to conceiving innovative and regenerative approaches to economic growth while emphasising the sustainable use of the ocean to foment long-term sustainability and prosperity for the whole within the planetary boundaries, contributing to climate change mitigation and adaptation.

The ADT4Blue project (Advanced Digital Technologies for the Blue Economy) was devised to develop, implement, and scale business ideas addressing Blue Economy challenges through the application of advanced digital technologies while adopting best practices and focusing on data-value chains.

Advanced Digital Technologies will be instrumental to overcome the challenges the Blue Economy is facing such as illegal fishing, pollution, CO₂ emissions, ecosystems destruction, climate change, governance, international cooperation, and equitable distribution of wealth. Blockchain will disrupt the Blue Economy, by fomenting an ecosystem-centric model, supporting the decarbonization of Blue Economy activities, decentralization, digitalization, democratization, supporting collaboration, encouraging new blue financing mechanisms geared towards regenerating ecosystems while supporting coastal communities to thrive, and promoting the emergence of innovative business models and new ways of doing business and interacting with customers.

The plethora of new ways of doing business propelled by the underlaying technology Blockchain, will foment innovative solutions and services, disrupt the Blue Economy, and support the fabric of regenerative entrepreneurs to develop non-linear approaches to growing businesses, responding to society and environmental needs, while thriving economically and will be essential to develop an Irish economy resilient to climate change, supporting Ireland's goal to become climate neutral by 2050.



Abstract

Indirect-based approaches to assessing the heating behaviours of occupants in residential
buildings

<u>AzimiSechoghaei, M.^{1, 2}</u>, Moran, P.^{1, 2, 3, 4}, Goggins, J.^{1, 2, 3, 4}

- 1. Civil Engineering, School of Engineering, University of Galway, Ireland.
- 2. MaREI Centre for Marine, Climate and Energy, Ryan Institute, University of Galway, University Road, Galway, Ireland.
- 3. ERBE Centre for Doctoral Training, University of Galway, University Road, Galway, Ireland.
- 4. Construct Innovate, University of Galway, University Road, Galway, Ireland.

INTRODUCTION

According to Ireland's Climate Action Plan 2024, carbon emissions from all energy-consuming sectors should be reduced by half by 2030 and net zero by 2050. Currently, 48% of carbon emissions from fossil fuels for heating are related to the residential sector. Within the residential sector, space heating is responsible for 75% of the total carbon emissions. Improved residential heating system performance without sacrificing occupant comfort is one solution to enhance energy efficiency in dwellings. Therefore, it is required to understand how building occupants heat their homes. The focus of this research is to develop a method to assess the heating behaviours of building occupants without directly monitoring the heating system.

MATERIALS AND METHODS

An indirect model based on Indoor Environmental Quality (IEQ) data was designed to discover a heating system's operation status in residential buildings. A generalised linear mixed model (GLMM) has been developed to utilise the minimum possible variables (e.g., room air temperature, humidity, etc.) to identify the outcome (operation mode of the heating system) with an acceptable accuracy rate.

RESULTS AND DISCUSSION

Figure 1 demonstrates the total hours of space heating system operation for nine houses based on heat pump data compared to predicted hours from January to December 2022 in four timestamps of 5,10,30, and 45 minutes. The initial results reveal that the data loggers' interval frequency can impact the predicted values' accuracy.



Figure 1: Comparison of predicted and recorded hours of space heating system in operation

Using room-temperature equations alone provides a significant difference between predicted and actual values. As a result, the next step is to add more predictive variables (e.g., humidity, daytime, outdoor temperature, Heating Degree Days, etc.) discussed in the literature review to accurately predict the hours space heating was on.



Abstract

A new BEMT model for analysing helical-bladed vertical axis wind and tidal turbines

Fereidoonnezhad, M¹, Leen, SB¹, Nash, S¹, Flanagan², T, McGarry P¹.

1. Collage of Science and Engineering, University of Galway ÉireComposites Teo., Údarás Industrial Estate An Choill Rua, Inverin, Galway

INTRODUCTION

2.

Designing tidal turbines is a challenging task due to the harsh environment and strong forces generated by tidal currents. Therefore, accurate and efficient modelling frameworks are needed to analyse and design complex blade geometries. Blade Element Momentum Theory (BEMT) is commonly used to analyse tidal turbines as it provides an analytical framework to model the hydrodynamic interaction between the turbine and fluid flow, which is more computationally efficient than CFD simulation. However, standard BEMT formulations are not suitable for accurately simulating complex blade geometries such as spiral or helical blade geometries.

MATERIALS AND METHODS

This study presents a modified BEMT formulation for analysing vertical axis tidal turbines (VATTs) with spiral blade geometries. The method accurately incorporates alterations in lift and drag forces due to the non-orthogonal orientation of the blade's leading edge with respect to the fluid velocity vector. The modified BEMT formulation was implemented in MATLAB and validated using experimental data for a VATT. The researchers then conducted a VATT design parametric study to investigate the relationship between blade helix angle and power output. In addition, The modified BEMT approach was extended to analyse turbine self-starting capability, which is advantageous in remote and small-scale tidal sites.

RESULTS AND DISCUSSION

The model predicted that the helix angle of the blade influences peak power output and peak TSR, and an increase in blade helix angle results in increased torque and reduced power fluctuations. Moreover, the model predicted that fluctuations in tangential and normal forces acting on the blade are reduced, which lowers the risk of blade fatigue failure. Helical blade turbines were found to have wider self-starting capabilities compared to straight blade turbines. The study demonstrates the usefulness of the modified BEMT approach in designing and analysing complex blade geometries in tidal turbines, and the importance of considering blade helix angle in maximizing turbine performance.



Abstract

OPPS4GPP: Opportunities for Green Public Procurement to improve implementation of
circular practice
Ahmed1, M.Z.1, O'Donoghue2, C.2, McGetrick, P.1
1. College of Science and Engineering, University of Galway, Newcastle, Galway, Ireland
2. School, Research group and/or Institute Affiliation of authors from other affiliations
ABSTRACT: The objectives of the Opps4GPP Project are to identify and examine opportunities for green public procurement (GPP) in Ireland, quantify the associated costs and benefits, and

green public procurement (GPP) in Ireland, quantify the associated costs and benefits, and disseminate findings to relevant public bodies and key stakeholders. The project is primarily, but not exclusively, focused on GPP in relation to public building projects. It will involve whole life cycle assessment (LCA) of case study public building projects, recommendation of GPP criteria and metrics for adoption in Ireland, and development of an innovation systems approach to critically evaluate and address implementation gaps in both GPP policy and practice in Ireland.



Abstract

Generating Haploid Inducer lines of Perennial Ryegrass using CRISPR-Cas9 Gene Editing <u>Moman Khan</u>, Nikita Gondalia, Luis F Quiroz, Peter C McKeown, Galina Brychkova & Charles Spillane School of Biological & Chemical Sciences and Agriculture & Bioeconomy Research Centre, Ryan Institute, University of Galway, Ireland

INTRODUCTION: Ireland's livestock dominated farming systems mainly rely on forage grasses, in particular perennial ryegrass (Lolium perenne), which is the underlying biomass supporting 80% of milk production by volume and 70% of meat production by weight, contributing significantly to the country's economy and export earnings. For sustainable intensification of food production in Ireland (i.e. more food per unit input, including land area) there is a need to develop varieties with higher yields per hectare. Despite the existence of heterosis effects in ryegrass gene pools, there are no robust systems for heterosis breeding in ryegrass to develop higher yielding F1 hybrid varieties. Conventional breeding of perennial ryegrass breeding approaches take at least 12 years to generate a variety with only 0.2-0.5% genetic gain. The advent of double haploid (DH) technology allows more rapid production of homozygous lines which have been deployed for heterosis breeding in many crop species. However, DH technology requires the induction of haploid plant production through a haploid induction (HI) system followed by reduplication of the haploid genome, which is currently not possible ryegrass. While DH production through in vitro anther culture was introduced in the 1970s, successful regeneration of perennial ryegrass has until now been very rare (Begheyn et al., 2016). The CRISPR-Cas9 technique has been used in other crop species to generate novel haploid inducer lines by targeted mutagenesis of pollen-specific genes, to induce HI via sperm cells (Kelliher et al., 2017; Liu et al., 2020). A key aim within this SFI funded research is to generate HI lines of perennial ryegrass using CRISPR-Cas9 as a tool for development of heterosis breeding strategies in this temperate forage crop species.

MATERIALS AND METHODS: 1) *In silico* analysis performed using the NCBI database for ortholog identification of *LpMTL* based on *ZmMTL* genes; conserved domains analysed using the Genome SMART website; 2) For qPCR analysis, RNA was extracted from the samples using standard TriZOL protocol followed by cDNA synthesis. Primers were designed using PRIMER blast NCBI web; and 3) CRISPR-Cas9 Plasmids were designed using a polycistronic tRNA-gRNA (PTG) strategy in one construct having Cas9, three gRNA for the gene of interest, reporter genes *RUBY* and *GFP* and verified by restriction digest.

RESULTS AND DISCUSSION: Three orthologous gene sequences of were identified in perennial ryegrass by *in silico* analysis. Relative transcript levels of mRNA were measured in five different ryegrass tissues (Fig. 1a). Two genes exhibited higher expression levels of mRNA specifically in pollen, confirming male gametophyte specificity. Building on this finding, CRISPR plasmids targeting these genes were designed. Further experiments are underway to generate an HI line that will not harbour either CRISPR-Cas9 cassettes nor marker gene RUBY (Fig. 1B). The novel plant lines will be confirmed by quantitative SNP genotyping and PCR for the loss of CRISPR-Cas9 cassettes and the loss of Ruby expression in embryos and validated for the haploid inducer line by crossing with tester lines. By using the CRISPR-Cas9 technique to develop HI lines , we will pave the way for heterosis breeding schemes in ryegrass to generate enhanced varieties with superior traits in a shorter period and thereby revolutionize ryegrass crop improvement.



Abstract

Numerical assessment of air entrainment process of a plunging jet
Lahiru, M.J.D ₁ , Felder, S. ₂ , Kramer, M. ₃ , Mannion, P. ₄ , Mulligan, S. ₄ , Clifford, E. ₁
1. School of Engineering, University of Galway, Galway, Ireland and Ryan Institute,
University of Galway, Galway, Ireland
2. VorTech Water Solutions Ltd., Galway, Ireland
3. Water Research Laboratory, School of Civil and Environmental Engineering, UNSW Sydney,
Australia
4. School of Engineering and Technology (SET), UNSW Canberra, Australia
Dividing liquid into constitute a cominal example of colf paration. They are often used in civil and

Plunging liquid jets constitute a seminal example of self-aeration. They are often used in civil and industrial applications, including wastewater treatment plants, weirs, spillways, and chemical mixing, while they can also be observed in natural settings, such as waterfalls and weir overflows. Research into this phenomenon is vital for the design and optimisation of water infrastructure.

In a plunging jet flow, atmospheric air is dragged along the jet into a receiving pool of water, generating a stream of self-entrained air bubbles into the water. The bubbles eventually reach a maximum depth, the penetration depth, before the bubbles start to rise due to buoyancy effects. During entrainment and rising motion, air bubbles tend to coalesce and break-up into a wide range of bubble sizes. Even though experimental studies of plunging jets have been abundant, numerical analysis has been limited, because of the complex multiphase nature of the flow, exhibiting a wide range of time and length scales. In recent years, a variety of two-fluid models has been implemented into numerical models and the accuracy of numerical methods has improved. Thus, numerical approaches have become viable for the investigation of complex two-phase flows.

In present literature on numerical modelling of plunging jets, the initial impingement of the jet flow has not been quantitatively investigated and validated. At the same time, the availability of various numerical models poses the question on their selection, based on accuracy and computational requirements. This work combines experimental and computation approaches to improve the modelling of plunging liquid jet flows, which is anticipated to lead to design improvements, contributing to more sustainable and resilient water infrastructure.



Abstract

Evaluating the householder's retrofit journey: Findings from in-depth interviews with householders in Ireland McGinley, O. 1 1. Civil Engineering, School of Engineering

Ireland has ambitious targets for substantial retrofitting of existing dwellings, including retrofitting 500,000 existing dwellings to a B2-Building Energy Rating (BER) or better by 2030. This requires many homeowners to retrofit their homes, and the alleviation of significant retrofit barriers. An understanding of the householder retrofit decision-making process is therefore important for the design of policies that enable householders to retrofit. Current understandings of householders' retrofit decisions are, however, limited by their depiction as static decisions, rather than the outcome of a householder's progression through a multi-stage retrofit journey.

This paper presents the findings of in-depth interviews with 17 homeowners in Ireland, which evaluated the householder retrofit journey in detail, including the drivers which motivated householders' stage-to-stage progression through this retrofit journey, and the barriers faced. A conceptual model of the retrofit journey is presented.

A broad range of factors influenced householders' progression through each stage of the retrofit journey, with the factors that encouraged householders to embark on the retrofit journey, differing from those that influenced their plans and retrofit decisions. Additionally, the information sources householders contacted at each point in this retrofit journey changed as they progressed, while the time householders spent at any retrofit journey stage before progressing varied considerably. Thus, the research confirmed that policies can be more effective in encouraging retrofit uptake, where they are designed to address the key drivers and barriers that householders face at each stage of the retrofit journey. Policy recommendations are presented.



Abstract

High Entropy Oxides for green hydrogen production from anion exchange membrane (AEM) seawater electrolyzer

Selvam, Praveen Kumar¹, Riaz, Muhammed Sohail¹, Costa, Pau Farràs^{1*}

1. School of Biological and Chemical Sciences, University of Galway, Galway,

INTRODUCTION

One of the promising ways of producing green hydrogen is seawater electrolysis by anion exchange membrane (AEM) electrolyzer. Plenty of seawater (97%) is available in our world, which can produce hydrogen for the long term and at a low cost. Nevertheless, seawater also has many challenges. In particular, the overall reaction is influenced by the free energy of hydrogen adsorption, and the hydroxide precipitation in the cathode compartment blocks the electrode-electrolyte interface. Meanwhile, the chlorine evolution in the anode corrodes the anodic compartment, hindering the efficient production of hydrogen gas. However, suitable electrocatalysts for hydrogen and oxygen evolution reactions for saline water splitting have not yet been figured out.

MATERIALS AND METHODS

Here, we report a non-noble transition metal-based high entropy oxide nano electrocatalysts Ni_{0.2}Fe_{0.2}Cr_{0.2}Mn_{0.2}Ti_{0.2}O_x for hydrogen and oxygen evolution reactions in seawater electrolysis. The electrocatalysts were synthesized by using co-precipitation technique, further synthesized electrocatalysts were in-situ characterized in X-ray diffraction (XRD), scanning electron microscopy (SEM), Transition electron microscopy (TEM), Raman spectroscopy, and ex-situ characterized in linear sweep voltammetry (LSV), chronopotentiometry, and impedance studies.

RESULTS AND DISCUSSION





The synthesized HEO nanoparticles are coated on Ni foam, and Ti felt for cathode and anode to evaluate the electrocatalytic activity. Figures 1(a) and 1(b) shows that the electrocatalysts could achieve 10 mA cm⁻² at 321 mV and 416 mV for HER and OER in 0.1M KOH+0.5M NaCl, respectively. These research findings would uphold the possibilities of highly efficient green hydrogen production at low cost, sustainably, for the long term.



Abstract

"Assuring the chemical and microbial safety of organic waste spread on land in Ireland – metal(oid)s and nutrients"

Farid¹, S, Healy², M.G, Morrison¹, L

- 1. Earth and Ocean Sciences, Schools of Natural Sciences and Ryan Institute, University of Galway, Ireland.
- 2. Civil Engineering and Ryan Institute, University of Galway, Ireland.

PROJECT SUMMARY

Manure from animals such as cattle, sheep and chicken are used as organic fertilizers for sustainable agriculture. The application of animal manure improves the quality and productivity of crops by improving the physiochemical properties of soil. Although the land application of manure has significant positive impacts on plant growth, it may also result in elevated concentrations of metals and microplastics in both plants and soil, and have negative impacts on the human food chain, ecology, and biodiversity.

PROPOSED GOALS/OBJECTIVES

The overall objectives of this project are to provide quantitative data on the type, prevalence, and concentrations of chemical and biological hazards in organic waste spread on land in Ireland. This project will also identify the main risk pathways of loss of each hazard and will investigate the effectiveness of different strategies to mitigate against chemical hazards in the environment.

IMPACT

The outcomes of this project will inform farmers, anaerobic digestor operators, regulators, and other stakeholders about the hazards in organic wastes intended for land spreading in Ireland. In addition, it will provide guidance on best practice and policy for their control. This will provide empirical evidence underpinning various national and European policies on food safety and environmental protection such as Food Wise 2025, Common Agricultural Policy (CAP), European Green Deal , Farm to Fork Strategy and FSAI research priorities 2020, by ensuring that organic fertilizers are free of chemical and biological hazards. This will help protect food safety and public health.



Abstract

Resilient classrooms for the future – Exploring lean and agile techniques for sustainable and healthy learning environments
<u>Fathi, SF^{1,2,3}</u> , Kumar Mishra, AKM ^{4,5} , Goggins, JG ^{1,2,3,6}
1. School of Engineering, University of Galway, University Road, Galway, Ireland
2. ERBE Centre for Doctoral Training, University of Galway, University Road, Galway,
Ireland
3. MaREI Centre for Marine, Climate and Energy, Ryan Institute, University of Galway,
University Road, Galway, Ireland
4. School of Public Health, University College Cork, College Road, Cork, Ireland
5. DTU Sustain, Technical University of Denmark, Denmark
6. Construct Innovate, University of Galway, University Road, Galway, Ireland

Introduction

Classroom indoor climate refers to the indoor air quality (IAQ) and thermal environment component of the classroom's indoor environment. The indoor climate of a classroom affects student comfort and learning. Factors such as climate, building elements, HVAC system, and occupants and occupant behaviour has an intimate impact on classroom indoor climate. Classrooms need to be designed to face challenges to their indoor climate from these factors and continue functioning in an energy efficient manner. This would mean more conducive learning environments and less disruptions to teaching.

Methodology

To model these design principles for a classroom, a building performance simulation model was created for an existing classroom in Galway city. The construction details of the classroom were obtained from construction plans. The model for a single classroom was created using DesignBuilder software. Indoor air temperature (IAT), relative humidity, and CO₂ concentration level were considered as main parameters to assess indoor climate of the classroom.

Results and discussion

The energy model was calibrated using real data from the classroom, between February 2021 to June 2022. IAT and relative humidity of the classroom exported from DesignBuilder were compared with the logged temperature and humidity values. Following model validation, we would be evaluating different engineering solutions for indoor conditioning and ventilation to examine how they may be used to ensure energy efficient classroom with resilient indoor climate.



Abstract

Gaps in LCA practices for wood products between Ireland and worldwide <u>Ge, S.</u>, McGetrick, P.J., O'Ceallaigh, C. Timber Engineering Research Group & Ryan Institute, University of Galway

INTRODUCTION

Ireland committed to halving GHG emissions by 2030 from the 2018 levels and achieving net zero by 2050, where the building sector is allocated about 50% burden for carbon reduction. However, the predicted population increase by 2051 brings roughly 33,000 new home demands each year by 2040. Considering wood has already been identified as a low-carbon material, and the roundwood supply from Irish forests is forecasted to double from 2016 to 2035, timber is an excellent choice for balancing the housing demand and emissions requirement. Although the potential rise in carbon emissions can be minimised by applying timber in construction, the benefits are hard to quantify due to lacking comprehensive lifecycle data for Irish wood products. Moreover, the absence of related LCA regulations might limit the scale of timber application. Therefore, the SAOLWood project first identifies the gaps in LCA practices for wood products between Ireland and worldwide through a holistic review.

MATERIALS AND METHODS

The review covers Europe, Canada, the USA, Australasia, and Asia, and is conducted from macro and micro levels. At the macro level, international and countries' national LCA methodologies related to embodied carbon estimation are compared from (1) mandatory regulations, (2) time in force, (3) limit values, (4) national LCA database, and (5) LCA details. At the micro level, 5 EPDs for each product including sawn timber, MDF, OSB and CLT are collected, and the LCA information is compared from (1) LCA scope, (2) LCI analysis, (3) indicator assessment, and (4) interpretation.

RESULTS AND DISCUSSION

At the macro level, the Netherlands ranks first within Europe; it enforces LCA regulations and limit values for construction earlier than other countries (except for Germany), and its LCA quantification is more comprehensive since it covers all required modules for embodied carbon estimation and aggregates various climate impact indicators into shadow cost, while most countries only consider GWP. For Ireland, there is no customised national LCA methodology, although the IGBC is currently developing such a methodology. At the micro level, Ireland is under the average level in terms of LCA scope performance as 50% of total analysed EPDs cover all the required modules and 80% incorporate the environmental impacts from the wood waste treatment and corresponding benefits and burdens beyond the product life, but the EPD of MDF from MEDITE omit module D and the EPD of OSB from SMARTPLY only declares modules A1-A3. Regarding indicators, the GWP related to land use and land use change is waiting to be included in Irish EPDs. Moreover, the end-of-life (EoL) stage of Irish wood products is an assumed value due to the absence of more reliable data but initial studies would indicate that there is a significant discrepancy with reality. In the future, the review scope will be expanded, and more gaps will be identified.



Abstract

Development and Experimental Assessment of a Solar Tracker
<u>Fakhari, V.,</u> Finnegan, W.
Construct Innovate and the SFI MaREI Research Centre, Ryan Institute, School of Engineering,
University of Galway, H91 HX31, Ireland.

INTRODUCTION

In order to mitigate the pollution generated by fossil fuels, employing renewable resources of energy has garnered more attention in recent years. Among these, solar energy is one of the leading green energy sources that has great potential to produce electrical energy by employing photovoltaic technology. The efficiency of solar photovoltaic panels in generating electricity is directly related to the amount of radiation received from the sun. As the sun's position varies throughout the day, relative to the Earth, employing a solar tracker will improve the efficiency of electricity generation. The solar tracker follows the sun to ensure that the sun's rays are always perpendicular to the panel. In this research, a novel dual-axis solar tracker is designed, fabricated, and experimentally tested to assess its performance.

MATERIALS AND METHODS

Fig. 1(a) indicates the fabricated view of the solar tracker. This tracker comprises two DC motors to rotate the panel, optical sensors to identify the sun's location, and a microprocessor to implement a motion control strategy based on the feedback received from the sensors.





RESULTS AND DISCUSSION

The proposed tracker has been tested in a real-world environment compared with a fixed solar panel. Fig. 1(b) depicts the obtained results from the simulations and experiments for the netgenerated electrical power for both the tracker and fixed panel. This graph shows that the net produced energy by the tracker is 43.2% higher than the fixed panel during the day. This result suggests that employing a solar tracker will be promising to improve energy efficiency. Over the coming years, the authors intend to develop the next generation of the solar tracker, making it more effective and suitable for Ireland's environment.


Abstract

Re-blading of Irish Wind Turbines using Novel Technologies
Jiang, Y.1, Finnegan, W.1,2, Kelly, C.3, Flanagan, T.3, Ahmad, A.1, Goggins, J.1,2
1. SFI MaREI Centre, Ryan Institute, School of Engineering, University of Galway
2. Construct Innovate, University of Galway
3. ÉireComposites Teo, Co. Galway

INTRODUCTION

As the world moves towards a more sustainable way of life, Ireland must invest significantly in creating a carbon-free energy system. Currently, the largest source of renewable energy globally is from wind and Ireland has an installed capacity of wind energy of 4,137 MW, where 17% of wind turbines will reach their end-of-life by 2030. If solutions to extend turbine life are not found, 700MW of capacity will be decommissioned. To this end, this project aims to develop advanced technologies to retrofit aging turbines through re-blading with new highly efficient and resilient blades.

MATERIALS AND METHODS

There are two main steps involved in the blade design, namely the aerodynamic geometric design and the structural design. In the aerodynamic geometric design, the genetic algorithmbased optimisation is carried out to design the external geometry of the blade so it sees improved power production, compared to the original design. In the structural design, a screening method is employed to design the composite layup of the blade, with the aim to have increased stiffness and mass, compared to the original design.

RESULTS AND DISCUSSION

In this project, a highly efficient wind turbine blade was designed. Figure 1 compares the geometry and power production efficiency between the reference blade and the optimised blade. The optimised blade has 4.22% higher annual power production compared to the original design. The structural analysis revealed that a reduction of 12% in material usage is attained, while an improvement of 15% in blade stiffness has been achieved. By analysing the performances of the new blade design, it can be concluded that the methodology developed in this research is efficient in designing new blades for upgrading existing wind turbines.





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