Hybrid Model Digital Twin-Enabled Wearable Device Telerehabilitation Platform

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Keywords: Digital twinning, telerehabilitation, nonlinear modeling, AI, AR-XR

Telerehabilitation devices not only provide accessibility to healthcare technology for the low-income and elderly population but also provide a rich database for healthcare technologists and scientists. In this research, DT-enabled wearable biomedical devices will be used to acquire physiological and biomechanical information about the patient in an AR/XR environment supported by blockchain technology to secure patient information. Difficulties in designing such platforms are caused by real-time monitoring of critical physiological and biomechanical data with the DT approach. To the best of our knowledge, no platform can monitor central pulse pressure changes and predict possible risks via AI-enabled DT with AR/XR systems. The following milestones are planned for a successful AI implementation.

1. **Digital-Twin Model Design:** The success of a Digital Twin (DT) of any system relies on its model. Physics-based DT models have advantages over the only data-driven DT models because they inherently can predict the states of the systems even if there is no data available at the time. It is a known fact that modeling the kinetics of the human body locomotion is not trivial. Therefore, in this research, each extremity and the torso will be modeled separately, and HM-DTs will be designed for each body section.

2. **Wearable Device Design:** We propose HM-DT-enabled wearable biomedical devices that incorporate data-driven models with physics-based models. These devices comprise Inertial Measurement Units (IMU), accelerometers, and compasses to localize and predict the motion of the targeted section of the body. The HM-DT will be utilized by nonlinear system identification such as Nonlinear Auto-Regressive Moving Average with eXogenous input (NARMAX) and various filtering techniques such as Unscented Kalman Filter (UKF). This enables predicting the missing data in the case of any sensor failure in real time. In addition to tracking the motion of the body, physiological sensory augmentation will be provided by using additional sensors such as pulse pressure (PP), EEG, and body temperature sensors.

3. **AR/XR Platform Interfacing:** Developed HM-DT-enabled wearable devices will be used in the AR/XR platform to improve remote rehabilitation. Existing physio-rehabilitation protocols will be interfaced with the proposed AR/XR platform. Physical and biomedical data will be acquired with wearable devices during the application of the rehabilitation protocol. Adverse cardio-vascular events will be monitored by collected pulse pressure information in real-time.

4. **AI-Implementation:** Datasets collected from wearable devices and AR/XR platforms will be preprocessed and become AI-ready. Different scenarios will be generated for targeted rehabilitation cases including usage of Generative Evolutionary Future Extraction (GEFE), Generative Adversarial Network (GAN), and Deep Neural Networks (DNN).

ABSTRACT

Examining Environmental Equity Gaps in EV Charging Deployment

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Presentation Keywords - Electric vehicles, Equity, GIS, spatial analysis

The adoption of electric vehicles is on the rise with the need to reduce vehicle-related carbon emissions to combat climate change. This initiative has been fortified by proposals to establish 500,000 charging stations along the Interstate Road network in the United States, ensuring a 50-mile spacing between stations. Apart from the benefits to the EV owners through convenience, the deployment of these electric vehicle charging stations is expected to have an impact in the communities and locations in which they are placed through reduction of pollution, reduction of traffic noise and increase in employment opportunities. It is important for the deployment to consider the environmental justice impacts due to the regional demographic, environmental and socio-economic differences in different locations.

The aim of the study is to investigate through spatial modelling and data fusion, the gaps due to the existing deployments within South Carolina based on the environmental justice parameters. The study will use multi-scale geographic weighted regression and data analysis to examine the relationship between the two. The results of this study will be useful for decision-makers in guiding the inclusion of environmental justice parameters in the location of electric vehicle charging stations.

Multi-Sensor Integrated Simulation Environment for Methane Leak Detection Using Reinforcement Learning

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Keywords: Reinforcement Learning, Methane Detection, Environment Simulation, Unreal Engine, Microsoft AirSim, Sensor Fusion

Abstract

Technological progress has prompted the creation of complex simulation environments for various use cases. The study developed a dynamic simulation environment, integrating Microsoft AirSim (i.e., an open-source simulator for autonomous ground vehicles and drones) and Unreal Engine (an open-source 3D computer graphics game engine), in which we utilized several sensors on a drone to detect environmental methane leaks. The simulation environment developed in this study presents comprehensive environmental monitoring capabilities by integrating depth-based, RGB, and infrared cameras with light detection and ranging (Lidar) sensors.

The Unreal Engine simulates a methane leak, serving as a realistic scenario for data collection using sensors and methane leak detection algorithm development. The study also develops dynamic environmental conditions within the simulation environment, like snow, rain, and fog, to further replicate a real-world scenario that will help us assess the resiliency of our developed methane leak detection system against adverse weather conditions.

This project's primary goal is to use Reinforcement Learning (RL) algorithms to create an optimal policy allowing autonomous vehicles—such as cars and drones—to determine the waypoints from a predetermined source location to the methane leak site. The RL algorithm iteratively learns and improves its policy, leveraging the data collected from the simulation environment.

Furthermore, this simulation environment facilitates the development of a secure and affordable methane leak detection algorithm and serves as a validation platform before moving to real-world deployments. The simulation environment developed in this study fosters novel autonomous methane leak detection technologies by allowing controlled and repeatable testing of methane leak detection algorithms.

Deep Learning-Based Classification of Gamma Photon Interaction in Room-Temperature Semiconductor Radiation Detectors

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Keywords: Deep learning, Gamma-photon detection, radiation detection, Neural network

Abstract

Photon counting radiation detectors have become an integral part of medical imaging modalities such as Positron Emission Tomography or Computed Tomography. One of the most promising detectors is the wide bandgap room temperature semiconductor detectors, which depends on the interaction of gamma/x-ray photons with the detector material involves Compton scattering which leads to multiple interaction photon events (MIPEs) of a single photon. For semiconductor detectors like CdZnTeSe (CZTS), which have a high overlap of detected energies between Compton and photoelectric events, it is nearly impossible to distinguish between Compton scattered events from photoelectric events using conventional readout electronics or signal processing algorithms. Herein, we report a deep learning classifier CoPhNet that distinguishes between Compton scattering and photoelectric interactions of gamma/x-ray photons with CdZnTeSe (CZTS) semiconductor detectors. Our CoPhNet model was trained using simulated 662 keV samples to resemble actual CZTS detector pulses and validated using both simulated and experimental data. The model remarkably exhibited a 100% accuracy in predicting the type of interaction. These results demonstrated that our CoPhNet model can achieve high classification accuracy over the simulated test set. It also holds its performance robustness under operating parameter shifts such as Signal-Noise-Ratio (SNR) and incident energy. Our work thus shows a positive direction for developing next-generation high energy gamma-rays detectors for better biomedical imaging.

Electrochemical reactions of alcohols with small-membered ring systems for bioconjugation applications

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Keywords: Electrochemistry; Bioconjugation; Small-membered ring; Living cell labeling

With the increasing demand for controllable and practical methods that make the possible formation of a new bond under clean (no oxidant or reductant), mild (water-tolerant), and inherently tunable (turn on/off) conditions, electrochemical (E-chem) methods have been gaining considerable interest recently. They can be applied not only in organic synthesis but also in bioconjugation applications. While E-chem bioconjugation has proven effective in directly modifying proteins using mild and controllable conditions with various electron-rich synthetic moieties, these moieties may be too large to efficiently attach to biomolecules. Therefore, there is a growing need to explore synthetic moieties that are small enough, relatively stable in the cellular environment, and sufficiently active upon E-chem activation and apply them to the realm of bioconjugation. In this study, alcohols with small-membered ring systems were chosen as in vivo bioorthogonal tags based on research on cyclopropene and diazirine. The ring of this type of alcohol can be opened by selective oxidation of selected anions under low cell potential and aqueous conditions, affording functionalized ketones. These functionalized ketones can act as electrophilic warheads in vivo and specifically react with their partners, making them a useful tool for not only biomolecular labeling but also drug delivery and real-time cell imaging in vivo, thus demonstrating the power of E-chem-based bioconjugation chemistry.

Machine learning enhanced design of RNA-based fluorescent biosensors for the detection of the neurotransmitter dopamine

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Keywords: biosensor, RNA aptamer, dopamine, random forest

Dopamine (DA) is a neurotransmitter that plays a role in the regulation of physical and emotional well-being. Irregularities in DA production have been linked to several addictive behaviors such as smoking, alcoholism, and obesity, as well as neurodegenerative disorders like Parkinson’s disease. Early detection of DA abnormalities is paramount for the effective diagnosis and treatment of these ailments, while real-time imaging of DA could assist in the comprehension of their underlying mechanisms. As such, our project aims to design a DA-sensing RNA-based fluorescent (RBF) biosensor for initial in vitro experimentation and characterization. Using existing platforms, we can fabricate RBF biosensors that combine a ligand-sensing RNA aptamer with a fluorescent RNA aptamer to indicate the presence of biologically relevant molecules. Previous studies have used electrochemical and protein-based biosensors in the detection of neurotransmitters; yet, to our knowledge, no studies have developed a viable RBF biosensor for the detection of DA *in vitro* or *in vivo*. To date, we have designed, transcribed, purified, and tested the dopamine detection of eight sensor variants.

To aid in the development of viable sensors our project utilized the assistance of machine learning algorithms based on other RNA sensor experiments. The 102 published RNA sensor sequences were cataloged based on the following characteristics: melting temperature of the entire sensor and the length, entropy, change in free energy, hydrogen bonds, and melting temperature of the transducer sequence that connects the dopa and Spinach 2 aptamers. These thermodynamic parameters along with the fluorescence fold increase were input into a decision tree classification model to predict which of these parameters is most influential in producing a good sensor. This dataset was further used to predict the efficacy of novel sensor designs. The distinction between good and bad sensors was made at a 2-fold increase and a classification tree was constructed using 102 sensors, the model accuracy was found to be around .76 as measured by the area under the curve of the Receiver Operating Characteristics or about 76% accuracy rating when the AI tested itself against the 102 sensors that it could test against.

High-Entropy Oxide Lithium Ion Battery Anodes

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Presentation Keywords: High-Entropy Oxide, Oxygen vacancies, Anode, Li-ion batteries

Abstract.
High-entropy oxides (HEOs), known for their extensive compositional diversity, while maintaining a single phase, and tunable electrochemical properties, are emerging as promising anode material for lithium-ion batteries (LIBs). The challenge of sluggish kinetics during prolonged cycling, however, has hampered their widespread adoption. In this study, we address this limitation by introducing oxygen vacancies into a rocksalt HEO oxide ((MgCoNiCuZn)O) via calcination under Ar atmosphere, with a goal to enhance ion and electron mobility. This modification significantly improves conductivity and Li^+ ion diffusion kinetics compared to the original HEO material. As a result, the modified anode achieves an impressive specific capacity of 598 mAh/g at 0.1 A/g, maintaining 99% capacity after 85 cycles at 0.2 A/g. Even after 1900 cycles at 3 A/g, the material shows a capacity of 249 mAh/g. The results demonstrate that the introduction of engineered defects into HEOs can markedly improve the lithium storage efficiency, charge transfer, and diffusion kinetics, thereby improving the electrochemical performance. Our approach provides a scalable strategy and valuable insights for developing defect-engineered HEO LIB anodes.

AI-Enabled Construction of Aligned Collagen using Two-Photon Techniques

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Keywords Fibrillogenisis, Photoinitator, Biofabrication, Artificial Intelligence

Introduction: The present state of tissue repair and replacement is dominated by regenerative medicine-based tissue engineering techniques, most notably creation of aligned collagen scaffolds as a base for deposited cell growth to form a tissue in an incubator [1]. Numerous tissue types are composed of a highly ordered and aligned collagen fibril matrix arranged into larger parallel fiber bundles. This aligned collagen architecture, predominantly collagen type I, is essential for tissue function including intervertebral discs, tendons, ligaments, muscles, neurons, the cornea, etc. To achieve functional tissue reconstruction, numerous new and improved manufacturing techniques for aligned collagen scaffolds have been developed, including isoelectric focusing, electrospinning, microfluidics, freeze-drying, extrusion, cyclic stretching, and shear flow-induced crystallization [2]. Unfortunately, clinical application of a tissue engineered medical device has been disappointing, mainly because of local structural mismatch of the in vitro developed tissue. We conjecture that optical means of collagen alignment and controlled cell deposition are necessary and feasible to repair, rebuild and restructure highly ordered native tissue in situ. Here, we propose an artificial intelligence (AI) based innovative laser collagen alignment technique to be developed into an in-situ scaffold formation technology for producing the next generation of tissue engineering-based implantable biomedical devices.

Materials and Methods: Our laser-based collagen biofabrication process involves the use of a tunable 80 MHz femtosecond Ti:Saphire laser to optically generate a controlled and localized protein assembly known as fibrillogenesis, via a two-photon (2P) effect, into fibers and bundles. The process relies on the principle that collagen fibrillogenesis occurs when the net surface charge of collagen triple helices approaches zero. Proper distribution of charge along the collagen triple helix promotes the semihexagonal molecular structure necessary for the formation of collagen fibrils. To induce collagen fibrillogenesis, a photoinitiator capable of modifying the collagen triple helix charge is used. The charge change only occurs where the laser is scanned within the collagen-photoinitiator solution. A high-resolution translational stage is used in conjunction with the pulsed femtosecond laser to scan along a line to generate a highly aligned collagen fiber according to the vector paths generated by the AI model to create the desired features. The AI model generates vector paths of collagen networks that would be required to repair tissue such as at the site of an enthesis. Depending on the enthesis target tissue region, such as tendon/ligament, fibrocartilage, or bone regions on the enthesis, the laser may be scanned linearly, in a fan-like pattern, or in a criss-cross direction to induce collagen fibrillogenesis, mimicking the native fiber alignment essential for tissue functionality.

Results: Recently, using our 2P system, we were able to effectively produce laser generated collagen structures by moving the 2P laser beam through the custom collagen solution and irradiating specific locations that are generated from a 3D CAD model. We demonstrate a single layer of collagen bundles in the pattern of a square using diagonal lines as well as a nonlinear criss-cross pattern that forms a three-dimensional weaved mesh.

Further, we investigated how laser irradiation exposure affects precise control of the voxel and in turn, the fibrils, by systematically characterizing various laser speeds and powers to determine optimal assembly and alignment parameters.

Discussion and Conclusions: The presented laser-based collagen biofabrication process represents a significant advancement in the field of tissue engineering. The ability to induce collagen fibrillogenesis optically, with excellent spatial and temporal precision, offers a novel approach for generating customizable 3D collagen structures. Unlike other techniques that attempt collagen alignment of bulk solutions, our method achieves highly localized collagen assembly, allowing for the mimicking of even the most intricate native fiber alignment in tissues. The results obtained so far provide a foundation for future work in refining the laser parameters, exploring additional photochemicals for crosslinking, and expanding the range of 3D structures that can be generated. The combination of optical induction of collagen fibrillogenesis holds great promise for advancing the field of tissue engineering. Further investigations and optimizations will contribute to the development of highly customized and mechanically robust collagen-based tissues for various biomedical applications.

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