2021 Postdoc Research Symposium
12-Minute Research Talks
Physical Science & Engineering: Abstract Book

1. **Dr. Austin Valentine Angulo, Engineering Systems and Environment, Civil Engineering and Human Factors. "Validation of Virtual Reality Simulator with Real-World Observations for Pedestrian Safety at Midblock Crossings"**

Purpose: Pedestrian fatality rates have been increasing at alarming rates over the last decade and traditional methods of studying pedestrian safety are time consuming, costly, and reactive. Virtual reality (VR) simulators offer a proactive, cost effective, low risk platform for studying pedestrian behaviors within environments modeled to replicate real-world environments. Within these immersive virtual environments (IVEs), behavior with existing and alternative designs can be analyzed before implementation to assess the impacts these alternatives may have on safety and perception. This research presents a case study of pedestrian perceptions and behaviors with three mid-block crossing safety treatments – the "as-built" painted crosswalk, rapid flashing beacons, and a connected vehicle (CV) phone application – to demonstrate a VR simulation experimental design and framework for testing pedestrian safety treatments.

Methods: 117 real-world pedestrian's behavior was observed at the intersection of Water Street and 1st Street South in Charlottesville, Virginia (a crash "hot-spot" identified by the Virginia Department of Transportation). 50 study subjects were instructed to cross a one-to-one scale VR replication of the intersection of in VR with the three safety treatments.

Results: Pedestrian crossing behavior in VR was found to be similar to the as-built real-world intersection. Through post-experiment surveys, it was found that participants found the As-Built environment to be the least safe of the three treatments and that their sense of risk within the IVE was realistic. Generalized mixed models showed that both the flashing beacon and CV phone application were statistically significant in decreasing accepted gap size and crossing speed.

Impact: This study shows the potential for both stated preferences and measured behavior to be used for determining the implications of alternative roadway designs in VR simulation, providing a new tool for assessing and planning for pedestrian safety.

Developing and expanding simulator capabilities offers a novel and safe way to understand roadway operations and safety.

2. **Dr. Bishal Paudel, Biomedical Engineering, Systems Biology, Therapeutics, Pharmacology. "A sphingolipid-guided gene expression signature stratifies acute myeloid leukemia prognosis"**

B. Bishal Paudel*, Su-Fern Tan, Todd Lox, Wendy Dunton, Irene Lee, Tye Deering, Jeremy Shaw, Pedro Costa-Pinheiro, Myles Cabot, Francine Garrett-Bakelman, Kevin A Janes, Mark Kester, David Feith, Thomas Loughran.

Acute myeloid leukemia (AML) remains a clinical challenge, as standard therapy has not substantially improved in the past three decades. Although recent molecular profiling has yielded several genomic stratifications and targeted therapies used clinically, a majority of patients lack known mutations, and do not benefit from existing therapies. Therefore, there is anurgent need in improving risk classification that leads to novel therapeutics in AML. Accumulating evidence implicates a key role for dysfunctional sphingolipid metabolism in AML, raising the possibility for lipid-altering anti-cancer therapies. However, sphingolipid metabolic state is not immediately gleaned from genomic sequencing of samples. To determine whether sphingolipid profiles could stratify AML, we collected multimodal measurements centered on sphingolipid metabolic pathway. We quantified lipid, protein, RNA profiles in addition to key enzymatic activities on 30 human AML cell lines. Using integrative systems-biology approach, we identified two distinct lipid-based clusters in AML cell lines, Sphingomyelin^{High} (SM-H), and Glucosylceramide^{High} (GC-H), which are biologically significant and differ in enzyme activities.

Interestingly, two clusters differ in their sensitivity to lipid-targeting inhibitors, with SM-H cluster having less sensitivity (high-EC50) to drugs that lead to Ceramide accumulation than GC-H cluster. To identify gene signatures that define these lipid-based clusters, we performed inter- cluster differential gene expression analysis on transcriptomic data from Cancer Cell Line Encyclopedia. Using cluster-signatures, we stratified AML patients into high, and low groups, found that SM-H cluster signatures had poorer outcomes in both TCGA AML (169 patients), andBeatAML (254 patients) cohort. Taken together, these results suggest that sphingolipid-focused biomolecular measurements can functionally stratify AML cell lines. This approach coupled with genomic stratification could lead to new therapeutic options in AML, with potentials for drug combination strategies with lipid-targeting inhibitors. Future work will: 1.) expand the analyses toAML patient samples, 2.) test the functional significance of significantly associated genes.

3. **Dr. Mehrdad Dizaji Shafiei, Engineering Systems and Environment. "Adaptive Digital Twinning – An Immersive Visualization Framework for Structural CPS"**

Dr. Mehrdad S. Dizaji & Dr. Devin K. Harris,

This research investigates a high-risk/high reward scheme to technologize infrastructure systems by employing artificial intelligence-informed digital twins. The digital twinning of an infrastructure system establishes a collaborative feedback loop between the measurable data of the physical world and simulated processes in the virtual world, providing a domain-specific adaptation of the broader CPS framework necessary to inform decision-making. Applied to the domain of large-scale structural systems, this research evaluates the conjecture that immersive engagement using a digital twin representation of these structural systems will permit participants to observe, interact, and contextualize the complex behavior mechanisms associated with these systems in their operational environment. The research design investigates a series of technology innovations to assessing the hypothesis, incorporating AI models to imitate both simulation-based results and experiment-based measurements.

The model-based simulation and experimental characterization reformulations within the proposed digital twin framework require adapting simulation behavior and experimental measurements within a real-time collaboration environment. Therefore, to achieve a real-time collaboration environment, formulating an AI model to substitute the finite element modeling (FEM) computations by creating a model of the FEM outcomes and learning the highly complex mapping using deep learning neural networks is explored. Moreover, re-formulating a computationally expensive process using DIC to calculate structural deformation fields from image sequences using a deep learning neural network is investigated. While the base formulations (i.e., FEM and DIC) of these results are computationally expensive, the AI formulations generate the foundation for real-time interconnection between these results and also establish novel opportunities for integration within a visualization platform that is necessary for decision-making for large scale structural systems. Furthermore, to establish a real-time user-defined model tuning interaction within the visualization platform for decision-taking projections, it is essential to design an automated fast-strategy for fine-tuning the design variables for a real-time interface between the results from simulation-based AI and measurement-based AI. Therefore, an AI-based approach to substitute the finite element model updating (FEMU) strategy pivotal is formulated to optimize design variables using a deep learning neural networks architecture. After training all three AI models, a client-server-based architecture will be developed where a user can interact and calibrate with a finite element model of a structure in a computational server in a physical environment to diagnose, prognoses, and forecast the behavior of the structure based on alternative scenarios.

4. **Dr. Phong C.H. Nguyen, Data Science, Material science & Manufacturing, PARC: A Physic-Aware Recurrent Convolutional Neural Network for Hot Spot Dynamic of Shocked Energetic Material Assimilation**

Purpose: Heterogeneous energetic (HE) materials were proven to have microstructure-dependent properties; therefore, one could achieve desired explosion performance and safety by controlling their microstructures. However, this material-by-design process is confined by the time-consuming direct numerical simulation (DNS) in which the hot spot dynamic of HE materials is analyzed and the structure-property–performance (S-P-P) linkage is established. As a result, it is urgent to have an accurate and lightweight simulation method to replace DNS in the design optimization process.

Method: In this work, we proposed a novel physic-aware recurrent convolutional neural network (PARC) that can assimilate the hot spot dynamic during shock-to-detonation of HE materials with high fidelity. Unlike other machine learning (ML) based approaches, PARC is designed to strictly follow the nature of the hot spot dynamic; thus, it is more interpretable and more physic aware.

Result: The experiment results from a data set obtained from DNS with SCIMITAR3D have proven the capability of PARC in capturing the dynamic of hot spot ignition and growth during the shock-to-detonation process of HE materials. In addition, with the introduction of convolutional hidden states serving as high order representation of state functions, PARC's prediction results are more accurate in both hot spots identification and sensitivity evaluations. Moreover, the computational efficiency is drastically enhanced as the computation time is reduced from days on high-performance computers with DNS to minutes on a personal mid-end laptop with PARC

Impact: PARC can be used iteratively to analyze microstructures' performance during the optimization to reduce the computation time. Moreover, it can replace DNS for rapidly analyzing new microstructure designs or digital twin models of actual microstructures. Finally, with its saliency map, PARC could be utilized to identify the possible hot spot origins, which is extremely helpful in many applications of energetic materials such as safety management.