Artificially Intelligent Manufacturing Paradigm for Composites (AIM for Composites)
EFRC Director: Srikanth Pilla
Lead Institution: Clemson University
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Mission Statement: *To build an AI-enabled inverse design approach for fundamental understanding and integrated material-manufacturing design of advanced polymer composites for improved performance and energy-efficient manufacturing, thereby enabling a smaller carbon footprint, lower structural weight, and lower cost.*

Despite the vast design space of composites, there are significant gaps between the performance, economic and environmental targets, and current design and manufacturing approaches. Most egregious are the expensive, long development cycles and the sub-optimal design that waste resources and may adversely affect the environment and climate change. The fundamental cause of such gaps is the lack of detailed understanding of the influence of the material architecture, process methods, and parameters on material microstructure evolution and subsequently the end product's physical, economic, and environmental performance, which we refer to as the material-process-microstructure-performance (MP2) relationships. The current experimental or analytical material screening approach relies heavily on known material architectures and is a trial-and-error process which largely hinders the material design exploration and optimization capabilities. Such gaps motivate the discovery and construction of a physics-informed, AI-based, inverse design platform that centers on multiscale physics-based models that can capture and predict the parameter space of specific manufacturing processes and material characteristics during fabrication. We envision such a platform that will enable both the discovery of new composites materials forms and relevant new manufacturing methodologies.

The scientific goals of this cooperative research effort are: (1) to unravel the fundamental underpinnings of the MP2 relationship via constructing an uncertainty-aware multi-objective "Digital Life Cycle" (DLC) that represents a suite of seamlessly linked, experimentally converged, high-fidelity models embracing all stages of a composite component's life cycle, linking perceived risk from energy consumption to carbon footprint; (2) to leverage physics-informed AI models and build microservice-based cloud tools to enable inverse composites material architecture and manufacturing process design and in situ diagnosis and control; and (3) to inform and validate the DLC and AI models and implement new material and process designs by exploiting innovative material engineering, characterization, and testing methods. The scientific goals will be achieved via three research thrusts as shown in the three circles in Fig. 1. The green circle is the DLC representing a suite of seamlessly linked, high-fidelity multiscale models for simulating all stages of a polymer composite's life cycle, which also integrates uncertainty quantification and energy, environment, economy (E^3) impact evaluation. The DLC will enable the generation of a large quantity of high-fidelity data for the training of AI models. Equipped with the DLC-generated data, the AI modeling and inverse design research thrust (blue circle) will develop new AI models, including physics-informed neural networks (PINN) and multiscale deep

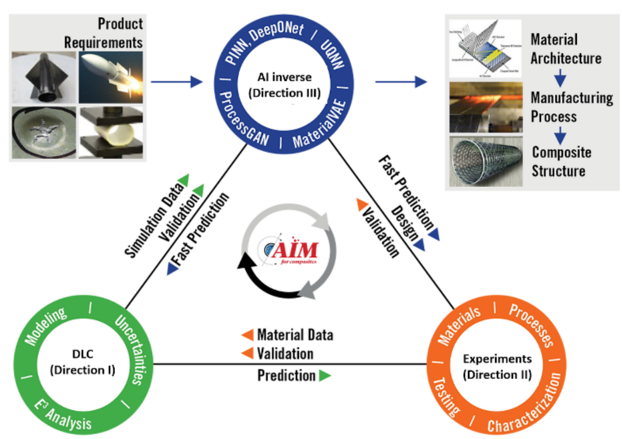

Figure 1. *Project overview: iterative loop among the DLC, AI modeling, and Experiments research thrusts, then AI models enable inverse design workflow.*

neural operators (DeepONet), to efficiently map composite materials' architecture and the manufacturing process to composite components' performance. Next, we will develop a conditional VAE neural network (MaterialVAE) for material inverse design and a conditional VAEGAN neural network (ProcessGAN) for manufacturing process design. Third, we will develop an uncertainty quantification neural network (UQNN) for in situ manufacturing diagnosis and control. By utilizing the experimental facility and capabilities at the University of Delaware's Center for Composite Materials, the University of Florida's Center for Manufacturing Innovation, the Pacific Northwest National Laboratory (PNNL), and other relevant BES facilities and infrastructure, we will conduct material characterization and testing of mechanical, physical, rheological, and morphological properties at nano-, micro-, and macroscales to inform and validate both DLC and AI models and simulations (orange circle). We will also implement new/hybrid processes that combine existing or new scalable processing routes to create tailored composite micro and macro structures. Finally, the inverse design is performed by the generative AI models. For given performance requirements, the material inverse design is first carried out using MaterialVAE to achieve the target material properties. For each material design candidate, and with the quality and E^3 impact requirements, the manufacturing process inverse design is performed using ProcessGAN. To further demonstrate and validate the DLC and AI models, we have recently incorporated testbeds (injection molding, thermoforming, and 3D printing) capable of fabricating varied geometries. Thus, the optimal composite material and its manufacturing process are obtained as a holistic solution.

Through the proposed research, the AIM for Composites EFRC aims to address the following challenges:

1. The models revealing the MP2 relationship need to capture the material behavior at multiple length scales (impurities, complex compositions), the effects of manufacturing processes (phase changes, non-equilibrium characteristics, E^3 impact), and both aleatory and epistemic uncertainties.
2. The possible material architectures and process conditions lead to a vast material and process design space with unknown boundaries and few data points, so it is challenging to determine the data sampling strategy and the volume of data to be generated for training ML models.
3. Integration of experimental characterization and testing with model development and validation.
4. How the physical principles will be preserved in ML models for them to represent nonlinear and transient functional properties.
5. Efficient and accurate models that enable in situ diagnosis and in-process decision making.
6. E^3 impact together with material property, manufacturing quality, and structural performance make the inverse design multiscale, multi-objective, and multidisciplinary.
7. Data fusion and flow among the DLC and ML models, experiments, and the inverse design steps.

Artificially Intelligent Manufacturing Paradigm for Composites (AIM for Composites)	
Clemson University	Gang Li (Associate Director), Zhen Li, Qiong Zhang, Mik Carbajales-Dale, Feng Luo, James Sternberg
University of Delaware / Clemson	Srikanth Pilla (Director)
Brown University	George Karniadakis (RT-2 Leader)
University of Florida	Young Huang (ECA Mentor)
Ohio State University	Farhang Pourboghrat (RT-1 Leader), Taejoon Park
South Carolina State University	Nikunja Swain, Biswajit Biswal, Ivan Radev
Savannah River National Laboratory	Dale Hitchcock
Pacific Northwest National Laboratory	Kevin Simmons (RT-3 Leader), Yao Qiao. David Mayberry, Daniel Merkel, Khaled Shahwan, Maria Swita

Contact: Srikanth Pilla, Director, spilla@udel.edu
302-831-3182, https://www.aimforcomposites.com/