APS Scientific Computation Seminar Series

Speaker:	Jeffery A. Aguiar, Ph.D. Research Scientist, Stf. Advanced Technology Center (ATC), Lockheed Martin Space
Title:	Automation at the Pace of Relevance and Speed
Date:	Monday, November 8, 2021
Time:	1:00 p.m. (Central Time)
Location:	Microsoft Teams meeting **Join on your computer or mobile app** Click here to join the meeting **Or call in (audio only)** +1 630-556-7958, 109947144# United States, Big Rock Phone Conference ID: 109 947 144# Find a local number | Reset PIN Learn More | Meeting options
Hosts:	Mathew Cherukara and Nicholas Schwarz

Abstract: One of the most active fields across all sciences and engineering disciplines is the use of information, knowledge, and computing to support informed decision-making. Whether it be controlling size, shape, and chemistry of nanomaterials, automating collection or analysis of on-the-fly data, the precise use of digitization and information networks are all equally challenging and at their equal forefronts. We now most importantly find ourselves where those same fundamental first-principles calculations and assumptions of microstructure and materials can now be altered and integrated with the addition of inference and experimental data. The accepted use of neural networks, machine learning and digital transformation has resulted in impressive advances for number of key areas, including new initiatives and directions across multiple fields of expertise utilizing new and unique facilities. In this talk, examples of answering historically hard grand challenge materials questions ranging from the phase and alteration of complex radioactive materials to pushing the on the fly of classifying crystallographic information will be presented with more than a notion of digital transformation at pace of relevance and speed.