

# CHEMICAL ENGINEERING

SEMINAR SERIES



**ROBERT RALLO**

**Monday, May 20, 2019**

Data Sciences

Advanced Computing, Mathematics, and Data Division  
Pacific Northwest National Laboratory

## **Data-driven analysis and modeling in Chemical and Environmental Engineering**

**ABSTRACT:** In this talk we will discuss diverse applications of data-driven techniques in Chemical and Environmental Engineering to illustrate the recent evolution in the field. First, we will discuss the challenges of early neural network and machine learning algorithms in two case studies related to the identification of coherent structures in turbulent flows and to the development of virtual sensors for product quality forecasting. The second part of the talk will focus on the application of machine learning techniques in environmental and process engineering, with examples in computational toxicology, environmental risk assessment and reverse-osmosis water desalination. The last part will discuss the application of deep learning techniques, highlighting current challenges and opportunities.

**RECEPTION 3:30 • LECTURE 4:00 – 5:00**  
**PHYSICS ASTRONOMY BLDG. PAA A 114**



**CHEMICAL ENGINEERING**  
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**BIOGRAPHY:** Since 2017, Dr. Rallo leads the Data Sciences Group in the Advanced Computing, Mathematics, and Data Division at Pacific Northwest National Laboratory. Prior to joining PNNL, he was an Associate Professor (2007-2016) in Computer Science and Artificial Intelligence and Director of the Advanced Technology Innovation Center (2012-2016) at the Universitat Rovira i Virgili, in Catalonia. During 2007-2008 and 2009-2011 he was visiting professor in the Department of Chemical and Biomolecular Engineering and in the California Nanosystems Institute at UCLA.

Dr. Rallo has been active in the broader scientific community by serving as chair of the Modeling WG for the European Commission Nanosafety Cluster (2012-2016) as well as EU co-chair for the Community of Research of Predictive Modeling for Human Health in the context of the US-EU Dialogue on nanoEHS (2013-2015). He also serves regularly as reviewer for the U.S. Department of Energy (DOE) and for several international research organizations including the European Research Council (ERC), the EU Horizon2020 Program, the COST Program and the NWO Research Council for Earth and Life Sciences (ALW).

His research interests focus on the applications of artificial intelligence at the intersection of chemistry, biology and computer science. His main scientific contributions have been in the areas of computational characterization of nano-bio interactions, nanoinformatics, computational toxicology and environmental engineering, and applications of data science and neural networks in engineering.