# IOWA

## **Multiscale** Computational **Science and Engineering**

The Multiscale Computational Science and Engineering Laboratory conducts research in areas of nanocomposites, robotics and control, and complex systems. The research group adopts advanced computational methods at different scales, including quantum mechanics, molecular dynamics, continuum mechanics, agentbased modeling, graph theory, and multiscale methods, enhanced by various artificial intelligence (AI) techniques such as deep learning and reinforcement learning.

#### Who We Work With

Laboratory

- Air Force Office of Scientific Research
- Iowa Initiative for Artificial Intelligence
- Iowa Institute of Hydraulic Research
- National Science Foundation



- Associate Professor of Mechanical Engineering, University of Iowa
- PhD: Mechanical Engineering, Northwestern University
- MS and BS: Modern Mechanics. University of Science and Technology of China



Technology

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## **RESEARCH** FOCUS & HIGHLIGHTS

**Multiscale modeling and simulation of nanocomposites:** To study the mechanics of nanocomposite, the lab developed a machine-learning-enhanced hierarchical multiscale model in which quantum mechanics, molecular dynamics, peridynamics, and finite element methods are employed at different scales. Neural networks are utilized to pass the information from one scale to another.

**Learning-based robotics motion planning:** The lab proposed a high-level control approach for robotics motion planning. The complex task is described by a formal language of linear temporal logics while the optimal policy is learned via reinforcement learning. In addition, infeasible missions are considered.

**Numerical and theoretical studies of complex systems:** Many complex systems can be modeled as networks. The lab proposed a memetic algorithm to design leader-follower networks for complex systems. On the other hand, the lab used an agent-based model to study COVID-19 outbreaks and outbreak control.

**Intelligent infrastructure systems:** Deep learning is used to generate a "digital twin" of the studied infrastructure system. Then, the best decision-making strategy can be obtained via reinforcement learning. The lab uses this approach to design a distributed reservoir system for flood mitigation and an intelligent traffic light system for traffic congestion reduction.

### LEARN MORE



SCHEDULE A VISIT

by contacting **Shaoping Xiao** at **shaopingxiao@uiowa.edu** or **319-335-6009** 



#### CONNECT WITH US

on our website iti.uiowa.edu/labs/multiscalecomputational-science-and-engineeringlaboratory

#### **Temporal Scale** Artificial Intelligence 1 year **Disease outbreak Biomechanics** 1 day**Quantum mechanics** 1 min**Molecular dynamics 1** *s* **Flood mitigation** $10^{-3}$ s Intelligent traffic light **Robotics and control** $10^{-9}$ s **Spatial Scale Nanocomposites** $10^{-12}m$ $10^{-6}m$ 1 km 1000 km 1m