

From Microscopic Structures and Dynamics to Macroscopic Functions in Complex Systems

Statement by Xiongye Xiao

Vision: My research is motivated by a central question in complex systems science: how do local interactions and multiscale organization give rise to emergent macroscopic function? Across natural and engineered systems, collective behaviors such as learning, synchronization, adaptation, and material functionality arise from structured interactions among many components. Yet despite decades of study, the mapping from microscopic structure and coupled dynamics to macroscopic function often remains qualitative and system specific. I seek to move this mapping from metaphor to measurement by developing mathematically grounded representations that render multiscale organization explicit, comparable, and learnable. By unifying structural geometry with operator-based modeling of dynamics, my work advances a structure–dynamics–function framework in which complexity is expressed not as intractable variability, but as a set of measurable organizing principles and generative rules. This perspective positions artificial intelligence itself as a complex system and aims to establish mathematical foundations for understanding emergent and trustworthy intelligence across biological and engineered domains.

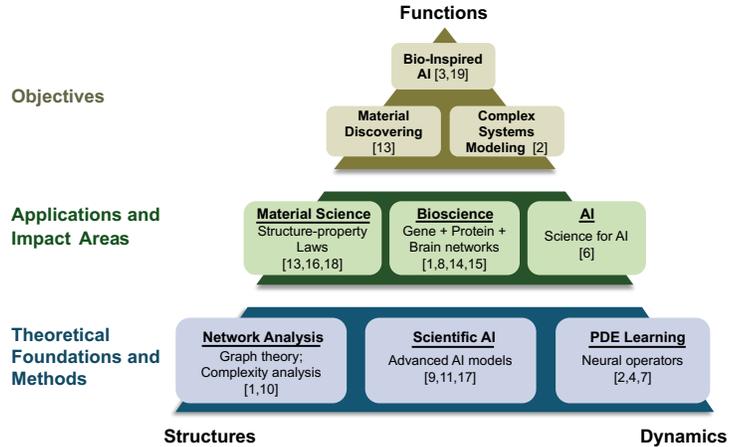


Figure 1: Overview of research framework: The pyramid illustrates my proposed theoretical foundations and methods (base); scientific applications and impact areas (middle), and objectives (top).

1. Original Contributions

Structure: Reframing Multiscale Organization in Complex Systems: A longstanding challenge in complex systems science has been the lack of quantitative descriptors capable of capturing multiscale heterogeneity beyond global graph statistics. Through the development of Node-based Multifractal Analysis (NMFA) [1,6], I introduced a mathematical framework that renders heterogeneous local interactions measurable at the level of individual units. Rather than summarizing networks through single-scale metrics, NMFA characterizes systems via node-resolved scaling laws and multifractal spectra, producing interpretable indicators of structural complexity, asymmetry, and cross-system distance.

This contribution moved network science forward by transforming multiscale organization from a qualitative observation into a measurable and comparable set of generative regularities. By uncovering structural generating rules underlying neuronal function [1,14] and providing quantitative guidance for microstructure-aware material design [10,13,16,18], NMFA reframed structural analysis as a rule-based, transferable methodology across domains, thereby establishing a new multiscale language for describing complex organization.

Dynamics: Reframing Multiscale Evolution as Learnable Operators: A central obstacle in complex systems science is the scalable modeling of strongly coupled, nonlinear multiscale dynamics. Traditional numerical solvers are computationally intensive and resolution dependent, while many data-driven approaches treat dynamics as trajectory prediction problems that do not generalize across scales. To address this gap, I developed multiwavelet-based neural operator frameworks [2,4,7] that learn evolution laws directly as operators between function spaces rather than as discrete time-step predictors. By operating in multiscale coefficient space, these models achieve resolution-invariant approximation while preserving both localized and global dynamical structure.

The Coupled Multiwavelet Neural Operator (CMWNO) [2] further reformulates interacting PDE systems into structured cross-scale mappings that are computationally scalable and physically interpretable, enabling efficient learning of strongly coupled multiscale dynamics. Extensions to nonlinear operator learning [7] improve robustness in high-dimensional and noisy regimes. This line of work moved scientific machine learning beyond black-box

simulation toward principled operator-level inference, establishing a transferable framework for modeling materials, fluids, and climate-related systems within the broader context of complex systems dynamics.

Function: From Multiscale Representation to Engineered Emergence: A fundamental challenge in complex systems science is that emergent macroscopic function is often treated as an outcome to be observed rather than a process to be systematically inferred. A central objective of my research has therefore been to translate multiscale structural and dynamical representations into predictive and engineering-relevant understanding of function. In neuroscience, NMFA uncovered structural generating rules associated with functional specialization and network robustness [1,14], reframing neuronal organization as a rule-governed architecture rather than a descriptive connectivity map. In materials science, multiscale network descriptors quantified how microstructural connectivity governs transport, mechanical response, and energy storage [10,13,16,18], enabling structure-guided design of high-performance systems [13] and demonstrating that material functionality can be engineered through principled structural modeling. In computational systems, extensions to weighted and directed graphs provided structure-aware metrics for heterogeneous hardware and large-scale AI models [5,6,8,12,19], linking structural self-organization to emergent computational behavior. Across these domains, my work moved complex systems research from observing emergence to formalizing and engineering it. By establishing computational mappings from multiscale organization and coupled dynamics to macroscopic behavior, it demonstrates that emergent function is not merely a byproduct of complexity, but a predictable and designable consequence of structured interactions across scales.

2. From Multiscale Organization to Engineered Emergence: A Reflection on Scientific Progress

Intelligence as Multiscale Emergence: How does intelligence arise from interacting components? I view intelligence not as an algorithmic artifact, but as an emergent macroscopic function of multiscale organization. Across biological neural systems and large language models (LLMs), intelligent behavior emerges from structured interactions evolving across scales rather than from parameter growth alone. My work identifies shared signatures of self-organization between brain networks and large-scale AI models [6,14], suggesting that intelligence is governed by measurable structural and dynamical principles that transcend substrate.

Building on this foundation, my future research aims to formalize these principles within a unified multiscale complex-network paradigm (Figure 2). By integrating geometric invariants that quantify organization across scales with operator-level models of collective evolution, I seek to identify the structural and dynamical regimes under which intelligence becomes robust, generalizable, and trustworthy.

This effort moves beyond empirical scaling toward engineered emergence, establishing a principled mathematical framework for understanding and designing intelligent systems.

Materials as Designable Complex Systems: Transformative progress in materials science requires moving beyond empirical structure–property correlations toward a predictive theory of multiscale organization. Real materials exhibit heterogeneous architectures across scales that challenge both traditional continuum descriptions and black-box machine learning models. A central scientific objective is therefore to identify transferable geometric and dynamical principles that govern how microstructural organization gives rise to macroscopic functionality.

Looking forward, I aim to develop a multiscale, network-based theory of materials in which functionality emerges from measurable structural invariants and constrained dynamical processes. By integrating graph-theoretic geometry, multifractal descriptors, and physics-informed operator learning, this framework will establish unified forward and inverse mappings between structure, dynamics, and property. Rather than treating materials discovery as data fitting, it seeks to enable rule-based, controllable, and interpretable design—advancing materials science toward engineered emergence grounded in mathematical principles.

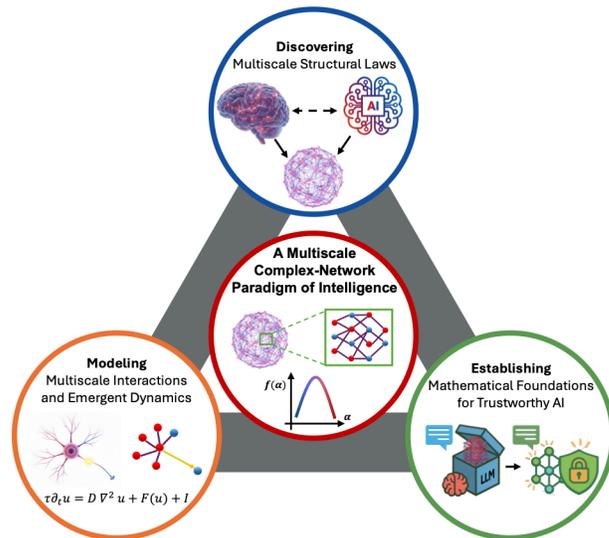


Figure 2: Structure, dynamics, and function paradigm for emergent and trustworthy intelligence.

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