

Research Interest

My research advances the foundational understandings of **large-scale complex systems** (e.g., social systems, infrastructure systems, multi-agent systems) through the lens of *machine learning*, *computational modeling* and *optimization*. I focus on developing **formal computational models and techniques** to simulate, analyze and optimize these large systems, with the goal of improving system performance and benefiting the **social good**. Particularly, I have performed abundant research in related issues such as improving fairness in social systems, resource allocation, multi-agent system planning, large-scale agent-based modeling, and black-box system inference.

Education

University of Virginia

Ph.D. Candidate in Computer Science (GPA: 4.0) - Advisor: Madhav Marathe

Charlottesville, USA

Aug 2020 – **Present**

Clemson University

M.S. in Computer Science (GPA: 3.75) - Advisor: Ilya Safro

Clemson, USA

Aug 2018 - May 2020

Southeast Missouri State University

B.S. in Computer Science (GPA: 3.7) - Dean's List, Cum Laude

Cape Girardeau, USA

Aug 2013 - May 2018

Research Projects and Papers

Project I: Optimal Resource Allocation on Large-scale Systems

Lead Researcher

Advisor: Prof. Madhav Marathe

- Project goal: **Design formal models and methodologies for optimal resource allocation on real-world large-scale systems.**
- Proposed formal frameworks for modeling resource allocation on large systems.
- Developed multiple efficient allocation algorithms that are *provably* optimal or near-optimal, while accounting for fairness and diversity.
- Conducted comprehensive agent-based simulations for resource allocation in large systems.

Project Outcomes:

[1] Welfare Optimization for Resource Allocation with Peer Effects

In Submission to PNAS

Zirou Qiu, Daniel Rosenkrantz, Matthew O. Jackson, Simon Levin, S. S. Ravi, Richard Stearns, Madhav Marathe

- We developed **a principled model for resource allocation with externalities** (e.g., mutual influences among the resources or the population) in real-world social and multi-agent systems.
- We proposed **efficient strategies** that guarantees **optimal or near-optimal** welfare outcomes for realistic resource allocation scenarios.

[2] Assigning Agents to Increase Network-Based Neighborhood Diversity [pdf]

AAMAS-23 (Acc: 23.3%)

Zirou Qiu, Andrew Yuan, Chen Chen, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, Anil Vullikanti

(Oral)

- We developed a formal model for real-world **spatial resources allocation** problems, such as public housing assignment and urban spatial planning.
- We presented **rigorous methodologies** for resource allocation with provable close-to-optimal guarantees, while achieving **social diversity and fairness**.

Project II: Efficient Inference of Large-scale Black-box Systems

Lead Researcher

Advisor: Prof. Madhav Marathe

- Project goal: **Develop efficient algorithms for learning unknown components in large-scale systems.**
- Proposed several efficient and highly scalable learning methods for black-box system inference.
- Established the performance guarantee of the proposed methods both theoretically and experimentally.

Project Outcomes:

[1] Learning Discrete Dynamical Systems under Classification Noise [pdf] **In submission to NeurIPS-2024**

Zirou Qiu*, Zakaria Mehrab*, Abhijin Adiga, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, and Anil Vullikanti

- We proposed **efficient noise-tolerant** algorithms for **learning the behaviors** of large-scale systems in realistic **noisy environments**, with a provable high learning accuracy.
- Our algorithms are highly **scalable to large networks**, and the amount of training data required is provable near-optimal.

[2] Theoretical Foundations for Parent Divorcing Transformations [pdf]

In submission to TCS

Daniel Rosenkrantz, ^(α - β) Madhav Marathe, **Zirou Qiu**, S.S. Ravi

- We established a theoretical groundwork for **dimensionality reduction in Bayesian inference**.
- We proposed **efficient algorithms** for dimensionality reduction with provable guarantees.

[3] Efficient PAC Learnability of Dynamical Systems Over Multilayer Networks [pdf]

ICML-24 (Acc: 27.8%)

Zirou Qiu, Abhijin Adiga, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, and Anil Vullikanti

- We proposed the first **efficient learning method** for inferring the behaviors of large-scale **multilayer** social systems and multi-agent systems.
- We lay a theoretical foundation of learning multilayer systems with an **exact analysis** of the model complexity and expressiveness.

[4] Learning the Topology and Behavior of Discrete Dynamical Systems [pdf]

AAAI-24 (Acc: 23.8%)

Zirou Qiu, Abhijin Adiga, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, and Anil Vullikanti

- We investigate the core principles of learning **both the behaviors and the topology** of black-box social systems and multi-agent systems.
- We proposed several **efficient learning algorithms** with provable guarantees for realistic scenarios of learning large systems.

[5] Learning Networked Dynamical Systems Via Active Queries [pdf]

ICML-22 (Acc: 22%)

Daniel Rosenkrantz, ^(α - β) Abhijin Adiga, Madhav Marathe, **Zirou Qiu**, S.S. Ravi, Richard Stearns, and Anil Vullikanti **(Spotlight)**

- We presented the first collection of **active learning** based methods for inferring **both the behaviors and the topology** of black-box social systems and multi-agent systems.
- We conducted an extensive experimental study on the empirical performs on the proposed algorithms on real-world networks over various learning scenarios.

Project III: Modeling and Simulation of Complex Systems

Lead Researcher

Advisor: Prof. Madhav Marathe

- Project goal: **Reveal novel phenomena and properties of large systems via (agent-based) simulation**.
- Designed principled models for multi-contagion diffusion on complex systems.
- Performed extensive simulations for dynamic processes over large systems on real datasets.
- Revealed novel phenomena and intrinsic properties of complex system dynamics.
- Derived policy guidelines for betterment of social good.

Project Outcomes:

[1] Airborne disease transmission during indoor gatherings over multiple time scales [pdf]

PNAS-23

Avinash Dixit, Baltazar Espinoza, **Zirou Qiu**, Anil Vullikanti, and Madhav Marathe

- We introduced **a principled modeling framework** that couples the fast dynamics of viral loads in the local scale and the slow dynamics of disease progression at the population level.
- We derived **policy guidelines** to lessen the negative impact of epidemics.

[2] Understanding the Co-evolution of Mask-wearing and Epidemics [pdf]

PNAS-22

Zirou Qiu, Baltazar Espinoza, Vitor V. Vasconcelos, Chen Chen, Sara M. Constantino, Stefani A. Crabtree, LuoJun Yang, Anil Vullikanti, Jiangzhuo Chen, Jörgen Weibull, Kaushik Basu, Avinash Dixit, Simon Levin, Madhav Marathe

- We presented a fundamental model for **dueling dynamics** of social and biological contagions both **cooperating and completing** in a population.

- Through our modeling, we uncovered a collection of previously unknown **phenomena** in contagion dynamics.
- We derived corresponding **policy guidelines** to suppress epidemics and prevent their resurgence.

Project IV: Dynamics and Stability of Complex Systems

Lead Researcher

Advisor: Prof. Madhav Marathe

- Project goal: **Investigate the foundations of stochastic behavior and stability of complex systems.**
- Conducted rigorous analytical studies of diffusion in complex systems.
- Performed extensive agent-based simulations of dynamic processes on complex systems.

Project Outcomes:

[1] Networked Anti-Coordination Games Meet Graphical Dynamical Systems [pdf] **AAAI-23** (Acc: 19.6%)
Zirou Qiu, Chen Chen, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, and Anil Vullikanti (Oral)

- We presented a theoretical groundwork for **stability and convergence** in real-world strategic situations such as **resources sharing and competition** within a society.

[2] Finding Nontrivial Minimum Fixed Points in Networked Dynamical Systems [pdf] **AAAI-22** (Acc: 15%)
Zirou Qiu, Chen Chen, Madhav Marathe, S.S. Ravi, Daniel Rosenkrantz, Richard Stearns, and Anil Vullikanti (Oral)

- We established the principles of finding **equilibrium points in contagion diffusion** within a population, with the goal of **minimizing the overall scale of infection** in a society.

Other Papers

[1] ELRUNA: Elimination Rule-based Network Alignment [pdf] **ACM JEA-2021**
Zirou Qiu, Ruslan Shaydulin, Xiaoyuan Liu, Yuri Alexeev, Christopher S. Henry, Ilya Saфро

- We propose novel algorithms for the **network alignment** problem that outperforms the state-of-the-art methods, with applications in computational biology and social network analysis.

Research Experience

Biocomplexity Institute and Initiative

Research Assistant

Advisor: Madhav Marathe; Mentors: S. S. Ravi, Dan Rosenkrantz

Fall 2020 – **Present**

- Investigated the foundations of social systems and multi-agent systems from the perspective of computational modeling, optimization, machine learning, and game theory.
- Developed large-scale frameworks for socio-technical system modeling.
- The lead researcher for four research projects, all resulted in multiple publications.
- Eight published works (PNAS 22 & 23, AAMAS 23, AAAI 22, 23 & 24, ICML 22 & 24), plus three in-submission papers.
- Worked in a team with over 40 scientists from various domains such as CS, social science, and economics.

Clemson University

Graduate Research Assistant

Advisor: Prof. Ilya Saфро

Jan 2019 - May 2020

- Studied computational problems in quantum computing and biology.
- Built a pipeline for microbiome modeling. Discovered novel microbiome migration pattern.

Argonne National Laboratory - Data Science Division

Graduate Research Aide

Host: Chris Henry

Summer 2019

- Performed comprehensive analysis of microbiome data.
- Investigated the network alignment problem with applications in computational biology.
- One first-author published work at ACM-JEA.