

Curriculum Vitae

Bai XUE

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Professional Summary

I am currently a Distinguished Research Professor at the Chinese Academy of Sciences, based at the Key Laboratory of System Software, Institute of Software. I have held a Research Professor position since September 2021 and was promoted to this distinguished rank in March 2026. Since September 2024, I have also served as Deputy Director of the Key Laboratory of System Software.

I served as a Visiting Professor at the College of Computing and Data Science (CCDS), Nanyang Technological University (NTU), hosted by Prof. Luke Ong, from August 2025 to February 2026. Since April 2026, I have been serving as a Visiting Professor at CCDS, NTU, for a second research visit continuing through October 2026.

I received my B.Sc. degree from Tianjin University of Technology and Education in 2008, and Ph.D. degree from Beihang University in 2014.

Before joining the Institute of Software as an Associate Research Professor in November 2017, I worked as a Research Fellow at the Centre for High Performance Embedded Systems, Nanyang Technological University (May 2014 – September 2015), and as a Postdoctoral Researcher in the Department für Informatik, Carl von Ossietzky Universität Oldenburg (November 2015 – October 2017).

Research Areas

Formal Methods · Deterministic and Stochastic Dynamical Systems · Control Theory · Safe Reinforcement Learning · Autonomous and Learning-Enabled Systems · Trustworthy AI

Research Vision

My long-term vision is to establish rigorous mathematical foundations for trustworthy autonomous and learning-enabled systems operating under uncertainty. To achieve this, I aim to bridge formal verification, control theory, statistical learning theory, and reinforcement learning, developing scalable methods that offer provable guarantees of safety and reliability while remaining computationally practical. Ultimately, my research seeks to enable trustworthy AI systems that combine the flexibility of modern learning approaches with the formal assurances necessary for deployment in complex real-world environments.

Academic Appointments

- Distinguished Research Professor, Institute of Software, Chinese Academy of Sciences, March 2026 – Present
- Deputy Director, Key Laboratory of System Software, Chinese Academy of Sciences, September 2024 – Present
- Research Professor, Institute of Software, Chinese Academy of Sciences, September 2021 – Present
- Associate Research Professor, Institute of Software, Chinese Academy of Sciences, November 2017 – August 2021
- Postdoctoral Researcher, Carl von Ossietzky Universität Oldenburg, Germany, November 2015 – October 2017
- Research Fellow, Centre for High Performance Embedded Systems, Nanyang Technological University, Singapore, May 2014 – September 2015

Education

- Ph.D. in Applied Mathematics, Beihang University, 2014
- B.Sc., in Information and Computing Science, Tianjin University of Technology and Education, 2008

Research Contributions

Formal verification of autonomous systems is commonly approached through two complementary paradigms: barrier-certificate methods and reachability analysis. Barrier certificate methods avoid exhaustive exploration of the state space by transforming verification problems into function-construction problems, enabling scalable verification through optimization and certificate synthesis. In contrast, reachability analysis explicitly computes reachable sets to characterize system behaviors under uncertainties and disturbances. Both approaches traditionally rely on accurate system models. However, with the rapid growth of AI and learning-enabled systems, black-box systems have become increasingly common, making system models difficult to obtain. As a result, data-driven formal methods have become increasingly important. My research develops unified theoretical and computational frameworks spanning these directions, with emphasis on scalability, formal guarantees, and trustworthy learning-enabled systems operating under uncertainty.

1). Equation-Relaxation-Based Barrier Function Methods for Formal Verification

https://lcs.ios.ac.cn/~xuebai/publication_eq.html

Developed a unified framework for constructing barrier-like certificates through equation relaxation, establishing a principled connection between verification completeness and computational tractability. The framework yields (i) *sufficient and necessary conditions* for infinite-horizon safety and reach-avoid verification of stochastic discrete-time systems, as well as sufficient and necessary conditions for finite-time safety verification of deterministic continuous-time systems, and (ii) barrier-like certificate conditions for safety and reach-avoid verification of stochastic discrete-time systems that *eliminate restrictive invariance assumptions commonly adopted in the literature*, thereby substantially broadening the applicability of barrier-certificate-based verification methods. A recent comparative survey (Cao et al., Comparative Analysis of Barrier-like Function Methods for Reach-Avoid Verification in Stochastic Discrete-Time Systems, arXiv, 2026) identifies two of these barrier-like certificate conditions among the strongest existing approaches for stochastic discrete-time reach-avoid verification. In addition, this framework has enabled the development of rigorous verification methodologies for continuous-time stochastic systems, an area that remains relatively underdeveloped and presents significant theoretical challenges.

In addition, this line of work includes: infinite-time reach-avoid sets generation for continuous-time stochastic systems, infinite-time reach-avoid verification for continuous-time deterministic systems, finite-time reach-avoid verification for stochastic continuous-time systems, (controlled/robust) reach-avoid sets generation for discrete-time deterministic systems, and (robust) invariant sets generation for discrete-/continuous-time deterministic systems. More recently, the developed conditions have also been applied to controller synthesis and safe reinforcement learning, and have inspired barrier-like conditions for finite-time safety and reach-avoid verification of stochastic discrete-time systems.

Selected publications:

1. **Bai Xue**. Sufficient and Necessary Barrier-like Conditions for Safety and Reach-avoid Verification of Stochastic Discrete-time Systems. *Automatica*, 2026.
2. **Bai Xue**. A New Framework for Bounding Reachability Probabilities of Continuous-time Stochastic Systems. *Nonlinear Analysis: Hybrid Systems*, 2026.
3. **Bai Xue**, Naijun Zhan, and Martin Fränzle. Reach-Avoid Analysis for Polynomial Stochastic Differential Equations. *IEEE Transactions on Automatic Control*, 2024.
4. **Bai Xue**, Martin Fränzle, and Naijun Zhan. Inner-Approximating Reachable Sets for Polynomial Systems with Time-Varying Uncertainties. *IEEE Transactions on Automatic Control*, 2020.
5. Yonghan Li, Chenyu Wu, Taoran Wu, Shijie Wang and **Bai Xue**. Converse Barrier Certificates for Finite-time Safety Verification of Continuous-time Perturbed Deterministic Systems. *Systems & Control Letters*, 2026.

2). Set-Boundary Propagation Methods for Formal Verification

(https://lcs.ios.ac.cn/~xuebai/publication_sb.html)

By carefully exploiting the topological properties of dynamical systems, developed a reachability analysis framework based on set-boundary propagation, showing that evolving only reachable-set boundaries is sufficient to compute over- and under-approximations of reachable sets. The framework *improves computational efficiency and approximation tightness* for nonlinear and uncertain dynamical systems. These boundary-propagation techniques have been adopted to compute inner-approximations in the reachability tool CORA (please refer to “Kochdumper, Niklas, and Matthias Althoff. Computing non-convex inner-approximations of reachable sets for nonlinear continuous systems. *CDC2020*”), and have inspired extensions in TIRA (please refer to “Meyer, Pierre-Jean, Alex Devonport, and Murat Arcak. TIRA: Toolbox for interval reachability analysis. *HSCC 2019*”).

Selected publications:

1. Jianqiang Ding, Taoran Wu, Zhen Liang, and **Bai Xue**. PyBDR: Set-boundary based Reachability Analysis Toolkit in Python. *FM*, 2024.
2. Dejin Ren, Zhen Liang, Chenyu Wu, Jianqiang Ding, Taoran Wu, and **Bai Xue**. Inner-approximate Reachability Computation via Zonotopic Boundary Analysis. *CAV*, 2024.
3. **Bai Xue**, Qiuye Wang, Shenghua Feng, Naijun Zhan. Over- and Under-approximating Reach Sets for Perturbed Delay Differential Equations. *IEEE Transactions on Automatic Control*, 2021.
4. **Bai Xue**, Arvind Easwaran, Nam-Joon Cho, Martin Fränzle. Reach-Avoid Verification for Nonlinear Systems Based on Boundary Analysis. *IEEE Transactions on Automatic Control*, 2017.
5. **Bai Xue**, Zhikun She and Arvind Easwaran. Under-Approximating Backward Reachable Sets by Polytopes. *CAV*, 2016.

3). PAC-Based Verification for Data-Driven and Black-Box Systems

(https://lcs.ios.ac.cn/~xuebai/publication_pac.html)

Developed a PAC-learning-based framework for the formal verification and analysis of systems with unknown or black-box dynamics. The framework proposes novel PAC one-step and multi-step invariants *that can be maintained recursively online*, and integrates statistical learning theory, barrier certificates, and scenario optimization to provide finite-sample formal guarantees for learning-enabled systems.

Selected publications:

1. Taoran Wu, Dominik Wagner, Luke Ong, and **Bai Xue**. PAC Finite-Time Safety Guarantees for Stochastic Systems with Unknown Disturbance Distributions. *HSCC*, 2026.
2. Taoran Wu, Yilin Xue, Jingduo Pan, Dejin Ren, Arvind Easwaran, and **Bai Xue**. Convex Computations for Controlled Safety Invariant Sets of Black-box Discrete-time Dynamical Systems. *IFAC*, 2026.
3. Taoran Wu, Dominik Wagner, Jingduo Pan, Luke Ong, Arvind Easwaran, and **Bai Xue**. PAC One-Step Safety Certification for Black-Box Discrete-Time Stochastic Systems. *Arxiv*, 2025.
4. **Bai Xue**, Miaomiao Zhang, Arvind Easwaran, and Qin Li. PAC Model Checking of Black-Box Continuous-Time Dynamical Systems. *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, 2020.

Research Grants and Projects

- Task-driven Safe Reinforcement Learning (Basic Research Program of Institute of Software, CAS, 2024-2028)
- Trustworthy AI Algorithms under Open Environment (CAS Project for Young Scientists in Basic Research, 2022.8-2027.7)
- Safety Verification of Hybrid Systems (CAS Pioneer Hundred Talents Program, 2018-2023)
- Formal Verification of Task-driven Robotic Hybrid Systems (CCF-Huawei Formal Methods Innovation Research Funding, 2021-2022)
- Trust to Train and Train to Trust: Agent Training Programs for Safety-Critical Environments (Singapore Ministry of Education, with NUS, NTU, SMU, 2021-2025)

- Safety Assurance for Machine Learning in CPS (Singapore Ministry of Education, with NTU, Singapore and ASU, USA, 2020-2023)
- Formal Verification of Delayed Dynamical Systems and Hybrid Systems(National Natural Science Foundation of China (NSFC), General Program, 2019–2022)
- Research and Applications of Human-Like Task Planning, Reasoning, and Verification Systems(National Natural Science Foundation of China (NSFC), Key Program, 2019–2023)

Supervision

Current Students

Taoran Wu (PhD)
 Yiling Xue (PhD)
 Dejin Ren (PhD)
 Zhipeng Cao (PhD)
 Jingduo Pan (PhD)
 Weiru Cui (PhD)
 Haoyang Cao (MSc)

Alumni Placement

Chenyu Wu (JD.com)
 Wei Li (JD.com)
 Yonghan Li (Huawei)
 Shuyuan Zhang (UCLouvain)
 Changyuan Zhao (NTU Singapore)
 Jianqiang Ding (Aalto University)

Teaching

- **Reinforcement Learning**
 School of Intelligence and Technology, HIAS, University of Chinese Academy of Sciences
 Offered: Autumn 2022, Autumn 2023, Spring 2024, Spring 2025
- **Foundational Academic Skills Development Seminars**
 University of Chinese Academy of Sciences
 Offered: Autumn 2024

Professional Service

- FMCAD / HSCC/ICCPS / CAV / ICML 2026 - PC Member
- NeurIPS 2026 - Reviewer
- IEEE ITSC 2026 - Associate Editor
- IEEE ITSC 2025 - Associate Editor
- HSCC / ICCPS 2025 - PC Member
- IEEE ITSC 2024 - Associate Editor
- RTCSA / ATVA / HSCC 2024 - PC Member
- AAI 2024 - PC Member
- HSCC 2023 - PC Member
- Reviewer, Mathematical Reviews (MathSciNet), American Mathematical Society
- ...

Selected Publications

Journal Articles

1. **Bai Xue**. Sufficient and Necessary Barrier-like Conditions for Safety and Reach-avoid Verification of Stochastic Discrete-time Systems. *Automatica*, 2026.
2. **Bai Xue**. A New Framework for Bounding Reachability Probabilities of Continuous-time Stochastic Systems. *Nonlinear Analysis: Hybrid Systems*, 2026.
3. Yonghan Li, Chenyu Wu, Taoran Wu, Shijie Wang, **Bai Xue**. Converse Barrier Certificates for Finite-time Safety Verification of Continuous-time Perturbed Deterministic Systems. *Systems & Control Letters*, 2026.

4. **Bai Xue**. Finite-time Safety and Reach-avoid Verification of Stochastic Discrete-time Systems. *Information and Computation*, 2025.
5. **Bai Xue**, Naijun Zhan, Martin Fränzle, Ji Wang, Wanwei Liu. Reach-avoid Verification Based on Convex Optimization. *IEEE Transactions on Automatic Control*, 2024.
6. **Bai Xue**, Naijun Zhan, and Martin Fränzle. Reach-Avoid Analysis for Polynomial Stochastic Differential Equations. *IEEE Transactions on Automatic Control*, 2024.
7. **Bai Xue**. Reach-avoid Controllers Synthesis for Safety Critical Systems. *IEEE Transactions on Automatic Control*, 2024.
8. Zhen Liang, Dejin Ren, **Bai Xue**, Ji Wang, Wenjing Yang, and Wanwei Liu. Verifying Safety of Neural Networks from Topological Perspectives. *Science of Computer Programming*, 2024.
9. Shuyuan Zhang, Lei Wang, **Bai Xue**, and Qing-Guo Wang. Automatic Verification of Bounded Synchronization for Heterogeneous Polynomial Networked Systems. *IEEE Transactions on Automatic Control*, 2024.
10. Shuyuan Zhang, Lei Wang, **Bai Xue**, Deyuan Meng, and Qing-Guo Wang. Consensus Criterion Verification for Heterogeneous Multi-Agent Systems via Sum-of-Squares Programming. *IEEE Transactions on Automatic Control*, 2024.
11. Qiuye Wang, Mingshuai Chen, **Bai Xue**, Naijun Zhan, and Joost-Pieter Katoen. Encoding Inductive Invariants as Barrier Certificates via Difference-of-Convex Programming. *Information and Computation*, 2022.
12. **Bai Xue** and Naijun Zhan. Robust Invariant Sets Computation for Discrete-Time Perturbed Nonlinear Systems. *IEEE Transactions on Automatic Control*, 2022.
13. Changyuan Zhao, Shuyuan Zhang, Lei Wang, and **Bai Xue**. Inner-approximating Robust Reach-avoid Sets for Discrete-time Polynomial Dynamical Systems. *IEEE Transactions on Automatic Control*, 2022.
14. **Bai Xue**, Qiuye Wang, Naijun Zhan, Shijie Wang, and Zhikun She. Synthesizing Robust Domains of Attraction for State-Constrained Perturbed Polynomial Systems. *SIAM Journal on Control and Optimization*, 2021.
15. **Bai Xue**, Qiuye Wang, Shenghua Feng, and Naijun Zhan. Over- and Under-approximating Reach Sets for Perturbed Delay Differential Equations. *IEEE Transactions on Automatic Control*, 2021.
16. **Bai Xue**, Martin Fränzle, Naijun Zhan, Sergiy Bogomolov, and Bican Xia. Safety Verification for Random Ordinary Differential Equations. *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, 2020.
17. **Bai Xue**, Miaomiao Zhang, Arvind Easwaran, and Qin Li. PAC Model Checking of Black-Box Continuous-Time Dynamical Systems. *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, 2020.
18. **Bai Xue**, Martin Fränzle, and Naijun Zhan. Inner-Approximating Reachable Sets for Polynomial Systems with Time-Varying Uncertainties. *IEEE Transactions on Automatic Control*, 2020.
19. **Bai Xue**, Arvind Easwaran, Nam-Joon Cho, and Martin Fränzle. Reach-Avoid Verification for Nonlinear Systems Based on Boundary Analysis. *IEEE Transactions on Automatic Control*, 2017.
20. **Bai Xue**, Zhikun She, and Arvind Easwaran. Under-approximating Backward Reachable Sets by Semialgebraic Sets. *IEEE Transactions on Automatic Control*, 2017.

Conference Papers

21. Jingduo Pan, Taoran Wu, Yiling Xue, and **Bai Xue**. Stochastic Minimum-Cost Reach-Avoid Reinforcement Learning. To appear in ICML'26.
22. Taoran Wu, Dominik Wagner, Luke Ong, and **Bai Xue**. PAC Finite-Time Safety Guarantees for Stochastic Systems with Unknown Disturbance Distributions. *HSCC*, 2026.
23. Taoran Wu, Yilin Xue, Jingduo Pan, Dejin Ren, Arvind Easwaran, and **Bai Xue**. Convex Computations for Controlled Safety Invariant Sets of Black-box Discrete-time Dynamical Systems. *IFAC*, 2026.
24. **Bai Xue**, Luke Ong, Dominik Wagner, and Peixin Wang. Refined Barrier Conditions for Finite-Time Safety and Reach-Avoid Guarantees in Stochastic Systems. *IFAC*, 2026.
25. Dejin Ren, Yilin Xue, Taoran Wu, and **Bai Xue**. Efficient Verification and Falsification of ReLU Neural Barrier Certificates. *AAAI*, 2025.
26. **Bai Xue**. Safe Exit Controllers Synthesis for Continuous-time Stochastic Systems. *CDC*, 2024.
27. Jianqiang Ding, Taoran Wu, Zhen Liang, and **Bai Xue**. PyBDR: Set-boundary based Reachability Analysis Toolkit in Python. *FM*, 2024.
28. Dejin Ren, Zhen Liang, Chenyu Wu, Jianqiang Ding, Taoran Wu, and **Bai Xue**. Inner-approximate Reachability Computation via Zonotopic Boundary Analysis. *CAV*, 2024.

29. Dejin Ren, Wanli Lu, Jidong Lv, Lijun Zhang, and **Bai Xue**. Model Predictive Control with Reach-Avoid Analysis. IJCAI, 2023.
30. Zhen Liang, Dejin Ren, Wanwei Liu, Ji Wang, Wenjing Yang, and **Bai Xue**. Safety Verification for Neural Networks Based on Set-boundary Analysis. TASE, 2023.
31. Yiqing Yu, Taoran Wu, Bican Xia, Ji Wang, and **Bai Xue**. Safe Probabilistic Invariance Verification for Stochastic Discrete-time Dynamical Systems. CDC, 2023.
32. Changyuan Zhao, Chuchu Fan, and **Bai Xue**. Outer-approximating Controlled Reach-avoid Sets for Polynomial Systems. CDC, 2022.
33. **Bai Xue**, Qiuye Wang, Naijun Zhan, Martin Fränzle and Shenghua Feng. Differential Games Based on Invariant Sets Generation. ACC, 2022.
34. Renjue Li, Pengfei Yang, Cheng-Chao Huang, Youcheng Sun, and **Bai Xue**, Lijun Zhang. Towards Practical Robustness Analysis for DNNs based on PAC-Model Learning. ICSE, 2022.
35. Qiuye Wang, Mingshuai Chen, **Bai Xue**, Naijun Zhan, and Joost-Pieter Katoen. Synthesizing Invariant Barrier Certificates via Difference-of-Convex Programming. CAV, 2021.
36. Pengfei Yang, Renjue Li, Jianlin Li, Cheng-Chao Huang, Jingyi Wang, Jun Sun, **Bai Xue**, and Lijun Zhang. Improving Neural Network Verification through Spurious Region Guided Refinement. TACAS, 2021.
37. **Bai Xue**, Yunjun Bai, Naijun Zhan, Wenyu Liu, and Li Jiao. Reach-avoid Analysis for Delay Differential Equations. CDC, 2021.
38. **Bai Xue**, Renjue Li, Naijun Zhan, and Martin Fränzle. Reach-avoid Analysis for Stochastic Discrete-time Systems. ACC, 2021.
39. Shenghua Feng, Mingshuai Chen, **Bai Xue**, Sriram Sankaranarayanan, and Naijun Zhan. Unbounded-Time Safety Verification of Stochastic Differential Dynamics. CAV, 2020.
40. Ting Gan, Bican Xia, **Bai Xue**, Naijun Zhan, and Liyun Dai. Nonlinear Craig Interpolant Generation. CAV, 2020.
41. Renjue Li, Jianlin Li, Cheng Huang, Pengfei Yang, Xiaowei Huang, Lijun Zhang, **Bai Xue**, and Holger Hermanns. PRODEEP: a platform for robustness verification of deep neural networks. ESEC/FSE, 2020.
42. **Bai Xue**, Naijun Zhan and Martin Fränzle. Inner-approximating Reach-avoid Sets for Discrete-time Polynomial Systems. CDC, 2020.
43. **Bai Xue**, Naijun Zhan, and Yangjia Li. Robust Regions of Attraction Generation for State-Constrained Perturbed Discrete-Time Polynomial Systems. IFAC, 2020.
44. **Bai Xue**, Naijun Zhan, and Yangjia Li. A Characterization of Robust Regions of Attraction for Discrete-Time Systems Based on Bellman Equations. IFAC, 2020.
45. Shenghua Feng, Mingshuai Chen, Naijun Zhan, Martin Fränzle, and **Bai Xue**. Taming delays in dynamical systems: Unbounded verification of delay differential equations. CAV, 2019.
46. **Bai Xue**, Qiuye Wang, Naijun Zhan, and Martin Fränzle. Robust invariant sets generation for state-constrained perturbed polynomial systems. HSCC, 2019.
47. **Bai Xue**, Martin Fränzle, and Naijun Zhan. Under-Approximating Reach Sets for Polynomial Continuous Systems. HSCC, 2018.
48. **Bai Xue**, Martin Fränzle, and Peter Nazier Mosaad. Just scratching the surface: Partial exploration of initial values in reach-set computation. CDC, 2017.
49. **Bai Xue**, Zhikun She, and Arvind Easwaran. Under-Approximating Backward Reachable Sets by Polytopes. CAV, 2016.

Preprints

50. Taoran Wu, Dominik Wagner, Jingduo Pan, Luke Ong, Arvind Easwaran, and **Bai Xue**. PAC One-Step Safety Certification for Black-Box Discrete-Time Stochastic Systems. Arxiv, 2025.
51. Zhipeng Cao, Peixin Wang, Luke Ong, Đorđe Žikelić, Dominik Wagner, and **Bai Xue**. Comparative Analysis of Barrier-like Function Methods for Reach-Avoid Verification in Stochastic Discrete-Time Systems. Arxiv, 2025.
52. Taoran Wu, Yiling Xue, Dejin Ren, Arvind Easwaran, Martin Fränzle, and **Bai Xue**. Controlled Reach-avoid Set Computation for Discrete-time Polynomial Systems via Convex Optimization. Arxiv, 2025.
53. **Bai Xue** and Luke Ong. Quantitative Verification of Finite-Time Constrained Occupation Measures for Continuous-time Stochastic Systems. Arxiv, 2026.
54. **Bai Xue**, Peixin Wang, and Luke Ong. Quantitative Verification of Constrained Occupation Time for Stochastic Discrete-time Systems. Arxiv, 2026.
55. Taoran Wu, Jingduo Pan, Luke Ong, and **Bai Xue**. Cost-Aware Adaptive Conformal Inference for Runtime Assurance in Dynamic Environments. Arxiv, 2026.