

Wuyue Yang (杨武岳)

yangwuyue@bimsa.cn | +86 18801273177

No. 544, Hefangkou Village Huaibei Town, Huairou District Beijing 101408

Professional Interests

My research focuses on the intersection of artificial intelligence and scientific discovery, with emphasis on:

- **Physics-Informed Machine Learning:** Developing interpretable neural network models that incorporate differential equations and physical principles
- **Scientific Machine Learning:** Creating AI methods for solving inverse problems in complex dynamical systems
- **Biomedical AI:** Applying data-driven approaches to biological systems, particularly protein aggregation dynamics and disease modeling
- **Collective Behavior Modeling:** Using machine learning to understand emergent properties in swarm systems and active matter
- **Knowledge-embedded Neural Networks:** Designing AI architectures that leverage domain knowledge for improved generalization and interpretability

Education

Ph.D. in Applied Mathematics, Yau Mathematical Sciences Center, Tsinghua University, Beijing, China 2017.9 –2022.6

- Thesis Title: Theory and Applications of Machine Learning Based on Differential Equations

B.S. in Mathematics, Department of Mathematical Science, Beijing Forest University, Beijing, China 2013.9 –2017.6

- Thesis Title: Kinetic Studies on the Regulation mechanisms of Inhibitors on the Amyloid Fiber Formation

Work Experience

Assistant Research Fellow, BIMSAs 2022.6 –Present

Publications

1. Shi Y, Yang W, Hong L. Extracting interaction kernels for many-particle systems by a two-phase approach. *Physics of Fluids*, 2025, 37(3). (Co-corresponding author)
2. Zhang X, Jia H, Yang W, et al. Thermodynamics for reduced models of polymer aggregation based on maximum entropy principle. *The Journal of Chemical Physics*, 2025, 162(16).
3. Zhang D, Yang W, Wen W, et al. A data-driven analysis on the mediation effect of compartment models between control measures and COVID-19 epidemics. *Heliyon*, 2024, 10(13). (Co-first author)
4. Fan G, Yang W, Wang D, et al. Prolonged lymphopenia and prognoses among inpatients with different respiratory virus infections: A retrospective cohort study. *Heliyon*, 2024, 10(11). (Co-first author)
5. Jiang Y, Yang W, Zhu Y, et al. Entropy structure informed learning for solving inverse problems of differential equations. *Chaos, Solitons & Fractals*, 2023, 175: 114057. (Co-first author, Co-corresponding author)
6. Li F, Yang WY, Ding MD, et al. A personalized pharmaco-epistatic network model of precision medicine. *Drug Discovery Today*, 2023, 28(7): 103608.
7. Hu P, Yang W, Zhu Y, et al. Revealing hidden dynamics from time-series data by ODENet. *Journal of Computational Physics*, 2022, 461: 111203. (Co-first author)
8. Yang W, Zhang D, Peng L, et al. Rational evaluation of various epidemic models based on the COVID-19 data of China. *Epidemics*, 2021, 37: 100501.
9. Li G, Zhou Y, Yang WY, et al. Inhibitory effects of sulfated polysaccharides from the sea cucumber *cucumaria frondosa* against A40 aggregation and cytotoxicity. *ACS Chemical Neuroscience*, 2021, 12(11): 1854-1859.

10. Yang W, Peng L, Zhu Y, et al. When machine learning meets multiscale modeling in chemical reactions. *The Journal of Chemical Physics*, 2020, 153(9): 094117.
11. Li G, Yang WY, Li WH, et al. Rational design of a cocktail of inhibitors against $A\beta$ aggregation. *Chemistry—A European Journal*, 2020, 26(16): 3499-3503.(Co first author)
12. Yang W, Tan P, Fu X, et al. Prediction of amyloid aggregation rates by machine learning and feature selection. *The Journal of Chemical Physics*, 2019, 151(8): 084106.
13. Li G, Yang WY, Zhao YF, et al. Differential Modulation of the Aggregation of N-Terminal Truncated $A\beta$ using Cucurbiturils. *Chemistry—A European Journal*, 2018, 24(51): 13647-13653. (Co first author)
14. Ran S, Huang T, Yang W. Tailored knowledge distillation with automated loss function learning. *PLoS One*, 2025, 20(6): e0325599. (Corresponding author)
15. Li G, Ran S, Yang W, Hong L. Improving generalization ability of deep-learning-based ODE solvers using continuous dependence. *npj Artificial Intelligence*, 2025, 1(1): 22. (Co-corresponding author)
16. Yang W, Peng L, Li G, et al. MEP-Net: Generating solutions to scientific problems with limited knowledge by maximum entropy principle. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 2025, 35(9).

Under Review

1. Mofidi H, Raissi M, Yang W. Exploring Multiple Timescale Dynamics Using Geometric Singular Perturbation-Informed Neural Networks (GSPINNs). *SIAM Journal on Scientific Computing*. (Co-corresponding author)
2. Jiang Y, Zeng Z, Yang W, Hong L, Zhu Y. Stwcr: Weak Collocation Regression for Revealing Hidden Stochastic Dynamics from Single Trajectory Data. (Submitted to *Journal of Computational Physics*)

Preprints

1. Yang W, Peng L, Zhu Y, et al. Identification of hydrodynamic instability by convolutional neural networks. arXiv preprint arXiv:2006.01446, 2020.
2. Peng L, Yang W, Zhang D, et al. Epidemic analysis of COVID-19 in China by dynamical modeling. arXiv preprint arXiv:2002.06563, 2020.

Peer review journals

1. Archives of Computational Methods in Engineering
2. Scientific Reports
3. Habitat International
4. AIMS Mathematics
5. International Conference on Learning Representations (ICLR)
6. Journal of Fuzzy Logic and Modeling in Engineering

Research Grants

1. National Natural Science Foundation of China (NSFC) - Youth Science Fund
 - Project Title: A Data-Driven Study on the Mechanism of Bacterial Cluster Dynamics (数据驱动的菌群集群动力学机制研究)
 - Role: Principal Investigator
 - Amount: 300,000.00 RMB
 - Period: 2024-01-01 to 2026-12-31
2. Commercial Aircraft Corporation of China (COMAC) - Beijing Civil Aircraft Technology Research Center
 - Project Title: Research on Aircraft Handling and Control Modeling Based on Machine Learning Inverse Problem Solving Methods (基于机器学习的反问题求解建模方法的飞机操稳控制建模研究)
 - Role: Principal Investigator

- Amount: 500,000.00 RMB
 - Period: 2025-04-30 to 2026-04-30
3. Ministry of Science and Technology (MOST) - National Key R&D Program
 - Project Title: Partial Differential Equation Modeling and Computation for Aircraft Engine Nacelle Problems (航空发动机短舱问题的偏微分方程建模与计算)
 - Principal Investigator: Yi Zhu
 - Role: Participant
 - Amount: 15,600,000.00 RMB
 - Period: 2021-12-01 to 2026-11-30
 4. Ministry of Science and Technology (MOST) - Consultant Project
 - Project Title: Advanced Mathematical Theory for Enhancing Artificial Intelligence Technology (以先进数学理论提升人工智能技术)
 - Role: Participant
 - Amount: 500,000.00 RMB
 - Period: 2025-03-01 to 2025-12-31
 5. Guangdong Provincial Key Laboratory of Dynamical Systems and Neural Systems
 - Project Title: "First Principles" and Data Dual-Driven Research on Alzheimer's Disease Dynamics ("第一性原理"和数据双驱动的阿尔兹海默症动力学研究)
 - Role: Participant
 - Amount: 100,000.00 RMB
 - Period: 2025-04-15 to 2026-12-15
 6. Beijing Municipal Natural Science Foundation - Haidian Original Innovation Joint Fund
 - Amount: 250,000.00 RMB
 7. National Natural Science Foundation of China (NSFC) - General Program
 - Project Number: 21877070
 - Project Title: Dynamic Study on the Regulation Mechanism of Protein Aggregation Inhibitors (针对蛋白质聚集的抑制剂调控机制的动力学研究)
 - Role: Participant
 - Amount: 540,000.00 RMB
 - Period: 2019-01-01 to 2022-12-31

Intellectual Property

1. Multi-organ Function Damage Identification System (多器官功能损伤识别系统)
 - Registration Number: 2024SR0421332
 - Type: Software Copyright
 - Year: 2024
2. Dynamic Identification and Classification System for Acute Kidney Injury Based on Sliding Time Window (基于滑动时间窗的急性肾损伤动态识别及分级系统)
 - Registration Number: 2023SR1325465
 - Type: Software Copyright
 - Year: 2023

Administrative and Service Work

1. Nominator for ICBS Speakers
2. Instructor at Beijing Summer Artificial Intelligence Training for Youth (2024)
 - Taught a course on PINN

3. Participated in the reception activities for visiting distinguished professor Adi Shamir during the ICBS.
4. Program Planning Committee Member
 - Participated in the planning of joint undergraduate AI talent cultivation program between Capital Normal University and Capital University of Economics and Business (参与 AI 中心人才联合培养项目规划)

Teaching and Mentoring

1. Doctoral Student Co-supervision
 - Supervised two doctoral students in joint training programs
2. Teaching
 - Taught 5 courses in Artificial Intelligence field :
 - Swarm Intelligence and Collective Behavior Dynamics (2025-02-18 to 2025-05-06)
48 hours, 21 students
 - Statistical Learning (2024-10-11 to 2024-12-27)
48 hours, 30 students
 - Collective Dynamics of Active Matter (2024-03-05 to 2024-05-21)
48 hours, 20 students
 - Complex System Dynamics and Control (2023-09-19 to 2023-12-14)
48 hours, 25 students
 - Topics on Sparse Identification of Nonlinear Dynamics (SINDy): Theory and Application (2023-03-14 to 2023-06-06)
48 hours, 30 students
3. Academic Seminars and Forums Organization
 - Organized 17 expert talks for BIMSA-Tsinghua Seminar on Machine Learning and Differential Equations (BIMSA-Tsinghua Seminar on Machine Learning and Differential Equations)
 - Organized 12 expert talks and internal discussions for BIMSA Thursday Machine Learning Applications Seminar (BIMSA Thursday Machine Learning Applications Seminar)
 - Organized Mathematical Biology and Deep Learning Forum with 10 expert talks