

Hongyu Yan

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EDUCATION

Xidian University (XDU) & Heriot-Watt University (HWU)

9/2020 ~ 6/2024

Joint Bachelor of Engineering in Telecommunications Engineering (GPA: 3.8/4.0, 89.6/100, top 10%)

- **Core Courses:** Mathematics for Engineering and Science (100/100), Mechanics and Waves (100/100), Introduction to Mechanical Engineering (99/100), Waves and Matter (97/100), Programming Practices (95/100), Digital Design and Programming (94/100), Introduction to Communications and Networks (97/100), Computer architecture and Embedded systems (95/100)

HONORS & AWARDS

- National Prize in “Challenge Cup” China Students Entrepreneurial Plan Competition 2022
- National Award in Computer Design Competition of Chinese College Students (Top 5%) 2022
- First Class Scholarship (Top 5%), XDU 2021
- Honorary Title for Outstanding Contributions to Internationalization, XDU 2021

PUBLICATIONS

- “PDMD: Potential-free Data-driven Molecular Dynamics for Variable-sized Water Clusters (H₂O)_{n≤21}”
(*Nature Communications*, Under review) – Frist Author
Arxiv: <https://arxiv.org/abs/2412.04442>
GitHub repository: <https://github.com/TACC/PDMD/tree/main?tab=readme-ov-file>
- Incremental Deployment Method of Segment Routing over an IPv6 (SRv6) Network Based on Graph Neural Network (GNN) and Multi-Agent Reinforcement Learning (MARL) (Patents)

PROJECTS & RESEARCH

PDMD: Potential-free Data-driven Molecular Dynamics for Variable-sized Water Clusters (H₂O)_{n≤21}

6/2023 ~ Present

Researcher | Advisor: Assis. Prof. Minghan Chen, Computer Science Department, Wake Forest University; Assis. Prof. Hanning Chen, Department of Chemistry, University of Texas at Austin; Prof. Yong Wei, Department of Computer Science, University of North Georgia

- Developed a potential-free data-driven framework for predicting system energy and atomic forces of variable-sized water clusters using Pytorch and PyTorch Geometric.
- Applied SOAP descriptor to generate high-dimensional, equivariant features about the atomic environment.
- Utilized ChemGNN, a graph neural network model that adaptively learns the atomic chemical environments without requiring a priori knowledge
- PDMD achieves a MAE of 7.1 meV/atom for energy and 59.8 meV/Å for forces, outperforming the state-of-the-art DeepMD by ~80% in energy accuracy and ~200% in force prediction.
- Proposed PDMD offers multiple-phase predictive power, enabling ultra-fast, general-purpose MD simulations while remaining *ab initio* accuracy.
- “PDMD: Potential-free Data-driven Molecular Dynamics for Variable-sized Water Clusters (H₂O)_{n≤21}”, under review in *Nature Communications*.

HI-MCALS: A Highly Interpretable Deep Learning Framework for Predicting Multi-Class Amyotrophic Lateral Sclerosis Images

9/2023 ~ 4/2024

Researcher | Advisor: Assis. Prof. Vallejo Marta, Heriot Watt University

- Developed the HI-MCALS deep learning framework to improve the diagnosis of ALS, a severe neurodegenerative disease with a high impact on patients' quality of life.
- Utilized data augmentation and transfer learning to address small dataset challenges.

- Enhanced model interpretability with Grad-CAM, providing visual explanations for diagnostic decisions.
- Achieved 89% diagnostic accuracy with the proposed model.

Incremental Deployment Method of Segment Routing over an IPv6 (SRv6) Network Based on Graph Neural Network(GNN) and Multi-Agent Reinforcement Learning (MARL)

1/2022 ~ 3/2023

Course Project | Advisor: Assis. Prof. Wenting Wei, Advanced Networking Technology Lab, XDU

- Investigated the solution for deploying SRv6 while maintaining traffic engineering optimization goals, modeling with edge as intelligent agent, using GNN for information transfer, obtaining link weights and selecting upgraded SR nodes based on the weights and graph theoretical knowledge.
- Improved the system generalization ability, training speed, using traditional algorithms combined with machine learning to select nodes for upgrade deployment in different IPv6 networks.
- Programmed experimental code in Python, PyTorch and Mininet, involving GNN networks, environmental building, modeling training, etc.

SKILLS & OTHERS

- **Programming Languages:** Python (Proficient), C, Java, PyTorch (Proficient), MATLAB (Basic)
- **Leadership Activities:** New Young Global Competency Development Program; Deputy Head of Technical Department of Technology Association; Minister of Environmental Protection Department of Caring Society
- **Talent:** Table Tennis (Won 1st prize in a college competition)