DEDI WANG

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EDUCATION

University of Maryland, College Park, MD, USA *Aug 2019-May 2024 (expected)*
PhD pre-candidate, Biophysics

Peking University, Beijing, China *Sep 2015-Jun 2019*
B.S., Physics GPA: 3.71/4.0

RESEARCH INTERESTS

Complex Systems, Molecular Dynamics Simulation, Enhanced Sampling,
Statistical Mechanics, Representation Learning & Artificial Intelligence (AI)

RESEARCH EXPERIENCE

Department of Chemistry & Biochemistry, University of Maryland *Sep 2019 – Present*
Research Assitant *Advisor:* ***Pratyush Tiwary***

- **Learning meaningful representations for molecular dynamics**
  Developed representation learning methods to speed up molecular dynamics simulations and make simulation data understandable for humans, applied them to a variety of systems, including the drug permeation through the phospholipid bilayer and pose changes in the medically relevant G-protein-coupled receptor (GPCR).

- **Open-source software for molecular simulations**
  Developed and maintained the codes of proposed methods in Github, provided mentorship and guidance to first-year graduate students and undergraduates in their research.
  Python code: **Github Link 1**, **Github Link 2**

Cancer Data Science Lab, NCI, NIH *Nov 2019 – Jan 2020*
Research Rotation *Advisor:* ***Sridhar Hannenhalli***

- **Identifying genes with distinct functions across different tissues**
  Applied the network diffusion to tissue-specific netwroks to get ”complete” tissue-specific GO annotations, developed a metrics to find out tissue-dependent genes which shed light on the underlying mechanism of some complex diseases.
  R code: **Google Drive Link** (unpublished)

Center of Quantitative Biology, Peking University *Jan 2017 – Jun 2019*
Undergraduate Research Assistant *Advisor:* ***Fangting Li***

- **The Global Dynamic Stability in Budding Yeast Cell Cycle**
  Built an auto-evolving simplified ODE model, developed new tools to analyze complex dynamic system, and proposed a promising mechanism that provides the cell-cycle process with a sufficient duration for each event and an attractive manifold for the state checking.
  C++ code: **Google Drive Link**

PUBLICATIONS

Wang, D., Wang, Y., Evans, L. and Tiwary, P., 2022. Introducing dynamical constraints into representation learning. arXiv preprint arXiv:2209.00905.

Vani, B.P., Aranganathan, A., **Wang, D.**. and Tiwary, P., 2022. From sequence to Boltzmann weighted ensemble of structures with AlphaFold2-RAVE. bioRxiv.

Mehdi, S., **Wang, D.**, Pant, S. and Tiwary, P., 2022. Accelerating all-atom simulations and gaining mechanistic understanding of biophysical systems through state predictive information bottleneck. Journal of Chemical Theory and Computation, 18(5), pp.3231-3238.

Wang, D., Zhao, R., Weeks, J.D. and Tiwary, P., 2022. Influence of Long-Range Forces on the Transition States and Dynamics of NaCl Ion-Pair Dissociation in Water. The Journal of Physical Chemistry B, 126(2), pp.545-551.

Wang, D. and Tiwary, P., 2021. State predictive information bottleneck. The Journal of Chemical Physics, 154(13), p.134111.

Wang, D., Zhao, Y., Zhang, Z., Lu, Y., Yang, X., Ouyang, Q., Tang, C. and Li, F., 2020. Critical slowing down and attractive manifold: A mechanism for dynamic robustness in the yeast cell-cycle process. Physical Review E, 101(4), p.042405.

MENTORING ACTIVITIES

Graduate students:

1. Jessica Bodosa
2. Shams Mehdi
3. Ryan Nival
4. Vanessa Meraz
5. Suemin Lee

Undergraduate student:

1. Fiona Mon

SELECTED HONORS AND AWARDS

Ann Wylie Dissertation Fellowship, University of Maryland, College Park	*Mar 2023*
Outstanding Research Assistant Award, University of Maryland, College Park	*Jan 2022*
Award for Scientific Research, Peking University	*Dec 2018*
May 4th Scholarship, Peking University	*Dec 2018*
Award for Academic Excellents, Peking University	*Dec 2017*
Award for Academic Deligence, Peking University	*Dec 2016*
May 4th Scholarship, Peking University	*Dec 2016*
Bronze Medal in the 31^{st} Chinese Physics Olympiad	*Nov 2014*

OTHER ACADEMIC ACTIVITIES

Brin MRC Workshop *Feb 2023*
Rare Events: Analysis, Numerics, and Applications

- Talk: ”Introducing Physics into representation learning”

Protein Folding Dynamics Gordon Research Conference *Oct 2022*

- Poster: ”Capturing Protein Conformational Dynamics through Information Bottleneck and Molecular Dynamics”

Protein Folding Dynamics Gordon Research Seminar *Oct 2022*

- Talk and poster: ”Capturing Protein Conformational Dynamics through Information Bottleneck and Molecular Dynamics”

American Physical Society March Meeting *Mar 2021*

- Talk: ”State Predictive Information Bottleneck”

Others:

Volunteer in MolSSI workshop on Machine Learning and Chemistry *Nov 2019*

Host student in Quantitative Biology 2018 conference of Peking University *Jul 2018*

Participant of the 7th Interdisciplinary Academic Forum of Peking University *Dec 2017*