Jiangyan Feng | Ph.D. Candidate

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Summary

- Forward-thinking computational biologist with 3+ years of experience in developing and using **atomistic simulation, machine learning, and data science approaches** for understanding complex biological processes, leading to **6 publications**.
- Excellent science communicator, both oral and written, leading to **multiple oral competition awards**.
- Self-motivated individual with easy-integration in a multicultural environment and proven ability to rapidly learn new problem domains by wining **multiple scientific competition awards**.

Skills

Technical Skills

- Expertized in all-atom molecular dynamics simulations, biased sampling methods including metadynamics and umbrella sampling.
- Expertized in stochastic modeling of time series, particularly in Markov modeling of complex protein dynamics from large-scale molecular simulations.
- Experienced in statistical analysis, such as direct coupling analysis and weighted histogram analysis method (WHAM).
- Experienced in high-performance computing, large-scale data analysis and modeling, and scientific visualization.
- Familiar with data mining, machine learning, and deep learning algorithms, and their applications in molecular simulations and protein dynamics.
- Familiar with theory and tools of bioinformatics.

Programming

- Experienced in Python, C/C++, Shell scripting
- Familiar with GPU programming, CUDA, MySQL, Java
- Exposure to MATLAB

Softwares

- Molecular modeling: Amber, Gromacs, OpenMM, NAMD, Rosetta, Schrödinger's Maestro
- Data analysis: Jupyter, NumPy, SciPy, Pandas, MDTraj, MSMBuilder, Osprey
- Machine learning: Scikit-learn, TensorFlow, Keras, DeepChem
- Visualization: PyMOL, VMD, Matplotlib, Origin
- Others: Git, LATEX, Microsoft Office, Octave

Projects: Computational Biology, Molecular Modeling, Machine Learning

Machine Learning for Protein Dynamics Prediction (ongoing)

- Developed a machine learning method for predicting alternative protein conformations through combination of agglomerative clustering and bioinformatics.
- Performed statistical analysis (direct coupling analysis) to extract evolutionary couplings from multiple sequence alignment.
- Related publication: **Feng J.** & Shukla D. (2018). Characterizing Conformational Dynamics of Proteins using Evolutionary Couplings. J. Phys. Chem. B. 122 (3), 1017-1025.
  Feng J. & Shukla D. (2019). FingerprintContacts: Predicting Protein Alternative Conformations from Coevolution. J. Phys. Chem. B. (submitted)

Automatic Feature Selection for Dimensionality Reduction

- Developed a genetic algorithm based technique to optimize feature selection for dimensionality reduction.

o Related publication: Chen Q.*, **Feng J.***, Mittal S. & Shukla D. (2018). Automatic Feature Selection in Markov State Models using Genetic Algorithm. J. Comput. Sci. Educ. 9 (2), 14-22. (* Equal contribution)

Pattern Discovery from DNA Sequences

o Developed a "motif finding" algorithm to discover patterns in DNA sequences.

o Codes are available at `https://github.com/JiangyanFeng-PhD/Motif_Finder`.

Molecular Dynamics Simulations of Nutrient Transport in Plants (ongoing)

o Performed large-scale all-atom molecular dynamics simulations on petascale supercomputer to unravel the molecular mechanisms of 3 different transporters.

o Constructed Markov state models to analyze time series simulation data and quantitatively characterized high-dimensional long timescale dynamics, thermodynamics and kinetics of plant and bacterial transporters.

o Employed genetic algorithm and dimensionality reduction techniques in feature search and selection, and utilized variational cross-validation to optimize parameters for Markov model constructions.

o Related publication: **Feng J.***, Chen J.*, Selvam B. * & Shukla D. (2019). Computational Microscope: Revealing Molecular Mechanisms in Plants Using MD Simulations. Plant Cell.

Education

Ph.D., Chemical & Biomolecular Engineering, University of Illinois, GPA: 3.78/4.00 — 2021
Concentration: Computational Science & Engineering, GPA: 4.00/4.00
M.S., Chemical & Biomolecular Engineering, University of Illinois — 2019
B.S., Chemical Engineering, Tianjin University, China — 2016, GPA: 3.83/4.00
Overseas Study, Western University, Canada — 2016

Publications

1. **Feng J.** & Shukla D. (2019). FingerprintContacts: Predicting Protein Alternative Conformations from Coevolution. J. Phys. Chem. B. (submitted)
2. **Feng J.***, Chen J.*, Selvam B. * & Shukla D. (2019). Computational Microscopy: Revealing Molecular Mechanisms in Plants using Molecular Dynamics Simulations. The Plant Cell. (* Equal contribution)
3. Chen Q.*, **Feng J.***, Mittal S. & Shukla D. (2018). Automatic Feature Selection in Markov State Models using Genetic Algorithm. J. Comput. Sci. Educ. 9 (2), 14-22. (* Equal contribution)
4. **Feng J.** & Shukla D. (2018). Characterizing Conformational Dynamics of Proteins using Evolutionary Couplings. J. Phys. Chem. B. 122 (3), 1017-1025.
5. **Feng J.**, Oyeneye O., Xu W. & Charpentier P. (2018). In-Situ NMR Measurement of Reactivity Ratios for Copolymerization of Methyl Methacrylate and Diallyl Dimethylammonium Chloride. Ind. Eng. Chem. Res. 57 (46), 15654-15662.
6. Wang S., **Feng J.**, Xie Y., Tian Z., Peng D., Wu H., & Jiang Z. (2016). Constructing Asymmetric Membranes via Surface Segregation for Efficient Carbon Capture. J. Membr. Sci. 500, 25-32.
7. Wang S., Tian Z., **Feng J.**, ... & Jiang Z. (2015). Enhanced CO_2 Separation Properties by Incorporating Poly (ethylene glycol)-containing Polymeric Submicrospheres into Polyimide Membrane. J. Membr. Sci. 473, 310-317.

Selected Honors & Awards

1. **Harry G. Drickamer Graduate Research Fellowship**, University of Illinois, USA — 2019-2020
2. **Area 53 International Speech Contest Second Place**, Toastmasters International, USA — 2019
3. **First Prize Poster Presentation**, University of Illinois at Urbana-Champaign, USA — 2018
4. **Third Prize**, Mathematical Contest in Modeling, USA — 2015
5. **Second Prize**, National Mathematical Contest in Modeling, China — 2014