NEGIN FOROUZESH

Ph.D., Assistant Professor

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SUMMARY

I am a tenure-track assistant professor in Computer Science at California State University, Los Angeles (Cal State LA). I develop novel approaches that synthesize physics-based computation and machine learning to enable modern drug design. I am a faculty member of the Biomedical Engineering (BME) minor program at Cal State LA, and an official developer of AMBER, an open-source software package for molecular dynamics simulation.

RESEARCH INTERESTS

- Biomolecular Simulation and Modeling
- Machine Learning
- Deep Generative Models
- High Performance Computing

EDUCATION

- **Ph.D. in Computer Science** 2015- 2020
  Virginia Polytechnic Institute and State University
  (Virginia Tech), Blacksburg,VA, USA
  Advisor: Dr. Alexey Onufriev
  Thesis: Efficient Biomolecular Computations Towards Applications in Drug Discovery
- **Master's Degree in Computer Science** 2011- 2013
  Amirkabir University of Technology
  (Tehran Polytechnic), Tehran, IRAN
  Advisor: Dr. Ali Mohades
  Thesis: Prediction of Protein Binding Sites Using Geometric Algorithms
- **Bachelor's Degree in Computer Science** 2007- 2011
  Amirkabir University of Technology
  (Tehran Polytechnic), Tehran, IRAN

PROFESSIONAL EXPERIENCE

- **Tenure-Track Assistant Professor** Aug. 2020- Present
  Computer science department at California State University, Los Angeles. Principle investigator of Computational Molecular Biology (COMB) Lab. We develop efficient computational models to simulate and analyze protein-ligand interactions.
- **Graduate Research Assistant** Jan. 2019- June 2020
  I worked on "Accurate Yet Fast Implicit Solvation" research project funded by NIH (R21) at Virginia Tech. My role was to perform optimizations on biomolecular surfaces to obtain an accurate estimation of binding free energies.
- **HPC Technical Support** Jan. 2018- Jan. 2019
  Advanced Research Computing (ARC), Virginia Tech
  I was mainly in charge of providing HPC consultancy and support for ARC users. Moreover, I built, tested and deployed software packages on clusters.
- **Biomedical Research Intern** May 2018- Aug. 2018
  Stanford Center for Genomics and Personalized Medicine (SCGPM), Stanford University

My role was to automate data import from large number of public annotation datasets to Google Cloud Platform (GCP) and keep the datasets up-to-date without human intervention.

GRANTS

- **(single PI): NIH SuRE FIRST R16**, "Improving the Accuracy of Implicit Solvents with a Physics-Guided Neural Network", 2022-2026, Total: $730,000
- **(co-PI): NSF PREC CHE Standard Grant**, "Cal State LA - MolSSI PREC Pathway to Diversity Program", 2022-2025, Total: $886,474.00
- **(single PI): NSF CISE IIS Standard Grant**, "Workshop on Computational Structural Biology 2021", 2021-2022, Total: $30,772
- **(single PI): CSUPERB New Investigator Grant Program**, "Computational Study of Novel Coronavirus Mutant Binding to the Human ACE2 Receptor", 2021-2022, Total: $14,997. Acceptance Rate: %36.
- **(co-PI): CSUPERB Curriculum Development Grant Program**, "An Introduction to Biomedical Engineering with Hands-On Design Projects", 2021-2022, Total: $14,999. Acceptance Rate: %36.
- **(single PI): XSEDE Startup Allocation**, "Improving the Accuracy of Molecular Docking with Physics-Guided Neural Networks", 2021-2022, Total: $3,670

AWARDS & HONORS

- **Graduate Student of the Year Award** Mar. 2020
  Recognized by the Virginia Tech Graduate School based on academic achievements, service contributions, and commitment to advancing women in science.
- **Computer Science Scholars and Pratt Fellowships** 2017, 2019
  Exceptional scholar admitted at Computer Science Department, Virginia Tech.
- **ACM Student Research Competition Award** Sept. 2018
  Third place in the Graduate Students Competition track, GHC 2018.

PUBLICATIONS

Peer-Reviewed Journals [* indicates the first student author]:

1. Case, D. A.,..., **Forouzesh, N.**, ... & Merz Jr, K. M. (2023). AmberTools. *Journal of Chemical Information and Modeling.* [IF: 5.6]
2. Cain*, S., Risheh, A., & **Forouzesh, N.** (2022). A Physics-Guided Neural Network for Predicting Protein–Ligand Binding Free Energy: From Host–Guest Systems to the PDBbind Database. *Biomolecules*, 12(7), 919. [IF: 5.5]
3. **Forouzesh, N.**, & Mishra, N. (2021). An Effective MM/GBSA Protocol for Absolute Binding Free Energy Calculations: A Case Study on SARS-CoV-2 Spike Protein and the Human ACE2 Receptor. *Molecules*, 26(8), 2383. [IF: 4.6]
4. **Forouzesh, N.**, Mukhopadhyay, A., Watson, L. T., and Onufriev, A. V. (2020). Multidimensional Global Optimization and Robustness Analysis in the Context of Protein-Ligand Binding. *Journal of Chemical Theory and Computation.* [IF: 6.006]
5. **Forouzesh, N.**, Izadi, S, and Onufriev, A. (2017, August). Grid-based Surface Generalized Born Model for Calculation of Electrostatic Binding Free Energies, *Journal of Chemical Information and Modeling.* 2017, 57, 2505-2513. [IF: 3.804]

Peer-Reviewed Conferences [* indicates the first student author]:

1. Sagar, D.*, Risheh, A., Sheikh, N., & **Forouzesh, N.** (2023, September). Physics-Guided Deep Generative Model For New Ligand Discovery. In Proceedings of the 14^{th} *ACM International Conference on Bioinformatics, Computational Biology, and Health Informatics* (pp. 1-9).
2. Rebel, A.*, Risheh, A., Massoudian, N., & **Forouzesh, N.** (2022, December). Calculating the Binding Entropy of Host-Guest Systems with Physics-Guided Neural Networks. *2022 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)* (pp. 3478-3485). IEEE.
3. Ramirez, S.*, Brieu, M., & **Forouzesh, N.** (2022, December). Low Data Image Analysis with a Generative Adversarial Network: A Case Study on Women Pelvic MRI Scans. *2022 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)* (pp. 2690-2695). IEEE.
4. Cain, S.*, Risheh, A., & **Forouzesh, N.** (2021, December). Calculation of Protein-Ligand Binding Free Energy Using a Physics-Guided Neural Network. *2021 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)* (pp. 2487-2493). IEEE.
5. Zhou, B.*, Mohammadi, F., Lim, J. S., **Forouzesh, N.**, Ghasemzadeh, H., & Amini, N. (2021). Analysis of macular thickness deviation maps for diagnosis of glaucoma. *In Advances in Visual Computing:* 16^{th} *International Symposium, ISVC 2021*, Virtual Event, October 4-6, 2021, Proceedings, Part II (pp. 53-64). Springer International Publishing.
6. **Forouzesh, N.** (2020, September). Binding Free Energy of the Novel Coronavirus Spike Protein and the Human ACE2 Receptor: An MMGB/SA Computational Study. In Proceedings of the 11^{th} *ACM International Conference on Bioinformatics, Computational Biology and Health Informatics* (pp. 1-7).
7. **Forouzesh, N.**, Watson, L. T., and Onufriev, A. V. (2020, May). Robustness of multidimensional optimization outcomes: a general approach and a case study. *2020 Spring Simulation Conference (SpringSim)* (pp. 1-12). IEEE.
8. **Forouzesh, N.**, Kazemi, M. R., and Mohades, A. (2014, June). Structure-Based Analysis of Protein Binding Pockets Using Von Neumann Entropy. *International Symposium on Bioinformatics Research and Applications* (pp. 301-309). Springer International Publishing.

Book Chapters & Editorials [* indicates the first student author]:

1. **Forouzesh, N.**, & Al Nasr, K. (2023). Special Issue "Protein Modeling and Simulation: Selected Articles from the Computational Structural Bioinformatics Workshop 2021". Biomolecules, 13(3), 408.
2. Mishra, N.* and **Forouzesh, N.**, 2022. Protein-Ligand Binding with Applications in Molecular Docking. In Algorithms and Methods in Structural Bioinformatics, Springer, 1–16.

PRESENTATIONS

1. The ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (ACM-BCB) Sep. 2023
   Houston, TX. [**Best Paper Finalist Award**]
2. The American Chemical Society (ACS) Fall National Meeting Aug. 2023
   San Francisco, CA
3. The Biophysical Society (BPS) Annual Meeting Feb. 2023
   San Diego, CA

4. The 12^{th} Southern California System Biology Symposium (SoCalSysBio 23) Apr. 2023
   University of Southern California, CA. [**Invited Speaker**]
5. The 5^{th} Southern California Theoretical Chemistry Symposium (SoCal TheoChem 5) Oct. 2022
   Riverside, CA. [**Invited Speaker**]
6. 36^{th} Annual CSU Student Research Competition May. 2022
   San Francisco, CA & Virtual. [**First Place Award**]
7. American Chemical Society (ACS) National Meeting Aug. 2021
   Atlanta, GA & Virtual
8. The American Chemical Society (ACS) Spring National Meeting Apr. 2021
   Virtual
9. The American Chemical Society (ACS) Spring National Meeting Apr. 2019
   Orlando, FL
10. Grace Hopper Celebration (GHC) of Women in Computing Sept. 2018
    Houston, TX. [**Best Paper Award**]
11. The American Chemical Society (ACS) Fall National Meeting Aug. 2017
    Washington D.C., VA
12. The 2^{nd} Molecular Biophysics Symposium Apr. 2017
    Virginia Tech Biocomplexity Institute, Blacksburg, VA
13. Computing Research Association- Women (CRA-W) Apr. 2017
    Grad Cohort Workshop, Washington D.C., VA
14. Drug Discovery Day Nov. 2016
    Virginia Tech Center for Drug Discovery (VTCDD), Blacksburg, VA

PROFESSIONAL MEMBERSHIP & SERVICE

Panels:

1. Ad-hoc Panelist of the Ohio Cancer Research 2023 Grant Review Summer 2023
2. Panelist of the NSF Biological Sciences (BIO) 2022
3. Panelist of the CSU Program for Education and Research in Biotechnology (CSUPERB) 2022
4. Ad-hoc Panelist of the NSF Computer and Information Science and Engineering (CISE) 2021

Organization:

1. PC Member of the Computational Structural Biology Workshop (CSBW) at ACM-BCB 2023 2023
2. Session Chair of the Artificial Intelligence Techniques for BioMedicine and HealthCare (AIBH) Workshop at IEEE-BIBM 2022 2022
3. Co-Chair of the Computational Structural Biology Workshop (CSBW) at IEEE-BIBM 2021 2021
4. Guest Editor of the MDPI Biomolecules, Special Issue: Protein Modeling and Simulation 2021-2022
5. Featured speaker at the Future Tech: Women in Tech 2021 2021

Membership:

1. Member of the Biophysical Society (BPS) 2022-
2. Member of the ACM Special Interest Group on Bioinformatics, Computational Biology, and Biomedical Informatics (SIGBio) 2020-
3. Member of the American Chemical Society (ACS) 2017-
4. Member of Association for Computing Machinery (ACM) 2016-
5. Mentor of the "Iranian Women in Computing (IranWiC)" 2018-
6. Treasurer of "Computer Science Grad Council at Virginia Tech" 2018- 2019
7. Treasurer of the "Iranian Society at Virginia Tech (ISVT)" 2017- 2018
8. Associate of "Virginia Tech Graduate Academy for Teaching Excellence" (VT-GrATE) 2019-2020

Reviews:

1. Reviewer of the "Machine Learning and the Physical Sciences" Workshop at NeurIPS 2023 2023-
2. Reviewer of the PLOS ONE Journal 2023-
3. Reviewer of the Machine Learning and HPC Track of SuperComputing Conference (SC'22). 2022
4. Reviewer of the Journal of Chemical Information and Modeling (JCIM) 2022-
5. Reviewer of the Journal of Molecular Biology (JMB) 2021-
6. Reviewer of the IEEE/ACM Transactions on Computational Biology and Bioinformatics (TCBB) 2021-
7. Reviewer of Journal of the ChemBioChem 2021-
8. Reviewer of the Journal of Computational Biophysics and Chemistry (JCBC) 2020-
9. Reviewer of the Journal of Computers in Biology and Medicine (CIBM) 2020-
10. Reviewer of Iranian Conference on Computational Geometry (ICCG) 2018

TEACHING EXPERIENCE

- Instructor
  - CS 4635: Modeling and Simulation, Cal State LA Spring 2023
  - CS 2148: Discrete Structures, Cal State LA Fall 2022
  - CS 2148: Discrete Structures, Cal State LA Fall 2021
  - CS 5112: Design and Analysis of Algorithm, Cal State LA Spring 2021
  - CS 2148: Discrete Structures, Cal State LA Spring 2021
  - CS 2148: Discrete Structures, Cal State LA Fall 2020
  - CS 3114: Data Structures and Algorithms, Virginia Tech Summer 2017
- Graduate Teaching Assistant
  - CS 5114: Theory of Algorithms, Virginia Tech Fall 2017
  - CS 4104: Data and Algorithm Analysis, Virginia Tech Spring 2017
  - CS 4104: Data and Algorithm Analysis, Virginia Tech Fall 2016
  - CS 5114: Theory of Algorithms, Virginia Tech Spring 2016
  - CS 4104: Data and Algorithm Analysis, Virginia Tech Fall 2015
  - Design and Analysis of Algorithms, Tehran Polytechnic Spring 2015
  - Design and Analysis of Algorithms, Tehran Polytechnic Spring 2012

- Certificates
  - Independent Improving Your Online Course (IYOC) Oct. 2021
    Quality Matters (QM)
  - DELTA New Faculty Institute Workshops Nov. 2020
    American Society for Engineering Education (ASEE)
  - Alt-Instruction Summer Institute Workshops July 2020
    Center for Effective Teaching and Learning (CETL) at Cal State LA

MENTORING & ADVISING

- Current Students, Cal State LA
  1. Ali Risheh, M.Sc. in Computer Science Fall 2022-
  2. Shivam Mishra, M.Sc. in Computer Science Fall 2022-
  3. Dikshant Sagar, M.Sc. in Computer Science Spring 2023-
  4. Ari Jasko, B.Sc. in Computer Science Summer 2023-
  5. Fergus Place, B.Sc. in Electrical Engineering Summer 2023-
- Alumni, Cal State LA
  1. Isabella Perez, B.Sc. in Biology Summer 2023
  2. Missael Corro-Flores, B.Sc. in Biophysics Spring 2023
  3. Nida Sheikh, B.Sc. in Computer Science Fall 2022- Fall 2023
  4. Alles Rebel, M.Sc. in Computer Science Spring 2021- Fall 2022
  5. Deepanker Seth, B.Sc. in Computer Science Fall 2022
  6. Negin Massoudian, M.Sc. in Electrical Engineering Spring 2022- Fall 2022
  7. Nikita Mishra, B.Sc. in Chemistry and Biochemistry Spring 2022
  8. Sahar Cain, M.Sc. in Computer Science Fall 2022
- Graduate Thesis Committees, Cal State LA
  1. Eric Chan, M.Sc. in Computer Science, Spring 2022
  2. Bingnan Zhou, M.Sc. in Computer Science, Spring 2021
  3. Veronica Toriz, M.Sc. in Computer Science, Spring 2021
  4. Kevin Delao, M.Sc. in Computer Science, Fall 2020
- Previously Mentored Students, Virginia Tech
  1. Dan Folescu, B.Sc. in Mathematics Summer 2019
  2. Karthik Ram, M.Sc. in Industrial Engineering Fall 2016
  3. Rohan Kaul, B.Sc. in Computer Science Spring 2016