NEGIN FOROUZESH

Ph.D., Assistant Professor

Email: neginf@calstatela.edu | Website: https://www.calstatela.edu/faculty/negin-forouzesh

SUMMARY

Tenure-track assistant professor in computer science at California State University, Los Angeles (CSULA). Apply physics-based and data-driven modelings, high performance computing (HPC) and machine learning techniques to simulate and understand biomolecular systems. With strong background in theoretical computer science, also have interests in design and analysis of algorithms and data structures.

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 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 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.
- **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 (SGCPM), Stanford University.
  I developed a database of genetic variant annotation on Google Cloud Platform (GCP), and the corresponding docker image.

HONORS & AWARDS

- **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** Sept. 2018
  Third place award in graduate students competition track, GHC 2018.

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PUBLICATIONS

Peer-Reviewed Journals and Conferences:

1. **Forouzesh, N.** (accepted). Binding Free Energy of the Novel Coronavirus Spike Protein and the Human ACE2 Receptor: An MMGB/SA Computational Study. In Proceedings of the *11th ACM International Conference on Bioinformatics, Computational Biology, and Health Informatics*.
2. **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*.
3. **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.
4. **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.
5. **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.

SELECTED PROJECTS

- **Global Optimization of Biomolecular Surfaces**
  Apr. 2017- Present
  Optimization of atomic radii in an implicit solvent model to obtain close agreement with experimental results in terms of calculating electrostatic binding free energies. The underlying massively parallel optimization method, VTDIRECT95, runs on Virginia Tech clusters.
- **Application of Deep Learning in Calculation of Binding Free Energies**
  Oct. 2019- Present
  Development of a physics-based deep learning network to calculate binding free energies of small protein-ligand complexes in an implicit solvent model. We build our model based on a machine learning framework called Deepchem, a python library mainly used in drug discovery processes.
- **Development of an Implicit Solvent Model in AmberTools**
  Jan. 2016- Apr. 2017
  Analysis and development of a grid-based surface generalized Born (GB) model, GBNSR6, for computing electrostatic solvation free energies of biomolecules. This model is freely available in AMBER package of molecular simulations.

PROFESSIONAL SERVICE/ MEMBERSHIP

- Reviewer, Journal of Computational Biophysics and Chemistry (JCBC), Oct. 2020
- Reviewer, Iranian Conference on Computational Geometry (ICCG), Jan. 2018
- Member, American Chemical Society (ACS), June 2017- Present
- Member, Association for Computing Machinery (ACM), Nov. 2016 - Present