

RAHMATULLAH ROCHE

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EDUCATION

Ph.D. in Computer Science and Applications Virginia Tech	August 2021 – Ongoing Blacksburg, Virginia, USA
Master of Science in Computer Science and Software Engineering Auburn University	August 2018 – August 2021 Auburn, Alabama, USA
Bachelor of Science in Computer Science and Engineering Bangladesh University of Engineering and Technology (BUET)	February 2011 – March 2016 Dhaka, Bangladesh

RESEARCH AND TEACHING EXPERIENCE

Research Assistant Advisor: Dr. Debswapna Bhattacharya, Department of CS, Virginia Tech <ul style="list-style-type: none">Employing deep learning techniques for predictive modeling	August 2021 – Ongoing Blacksburg, Virginia, USA
Research Assistant Advisor: Dr. Debswapna Bhattacharya, Department of CSSE, Auburn University <ul style="list-style-type: none">Developed methods for protein 3D structure predictionWorked on protein 3D structure visualization	August 2018 – July 2021 Auburn, Alabama, USA
Teaching Assistant Department of CSSE, Auburn University <ul style="list-style-type: none">Evaluated projects and assignmentsConducted question answering sessions and office hours	August 2018 – December 2020 Auburn, Alabama, USA
Lecturer Department of CSE, Eastern University <ul style="list-style-type: none">Taught core courses of computer scienceSupervised and monitored projectsPrepared report for quality assessment of education provided	September 2016 – July 2018 Dhaka, Bangladesh

REFEREED JOURNAL PUBLICATIONS

[1] **Rahmatullah Roche**, Bernard Moussad, Md Hossain Shuvo, and Debswapna Bhattacharya. E(3) equivariant graph neural networks for robust and accurate protein-protein interaction site prediction. *PLOS Computational Biology*, 2023.
<https://doi.org/10.1371/journal.pcbi.1011435>

[2] Bernard Moussad, **Rahmatullah Roche**, and Debswapna Bhattacharya. The transformative power of transformers in protein structure prediction. *Proceedings of the National Academy of Sciences* 2023.
doi: <https://doi.org/10.1073/pnas.2303499120>

[3] Sutanu Bhattacharya, **Rahmatullah Roche**, Md Hossain Shuvo, Bernard Moussad, and Debswapna Bhattacharya. Contact-Assisted Threading in Low-Homology Protein Modeling. *Homology Modeling: Methods and Protocols*, Springer US 2023 (Book Chapter).
doi: https://doi.org/10.1007/978-1-0716-2974-1_3

[4] Md Hossain Shuvo, Mohimenul Karim, **Rahmatullah Roche**, Debswapna Bhattacharya. PIQLE: protein-protein interface quality estimation by deep graph learning of multimeric interaction geometries. *Bioinformatics Advances*, 2023.
doi.org/10.1093/bioadv/vbad070

[5] **Rahmatullah Roche**, Sutanu Bhattacharya, Md Hossain Shuvo, and Debswapna Bhattacharya. rrQNet: Protein contact map quality estimation by deep evolutionary reconciliation. *PROTEINS: Structure, Function, and Bioinformatics*, 2022.

doi: <https://doi.org/10.1002/prot.26394>

[6] Sutanu Bhattacharya, **Rahmatullah Roche**, and Debswapna Bhattacharya. DisCover: distance- and orientation-based covariational threading for weakly homologous proteins. *PROTEINS: Structure, Function, and Bioinformatics*, 2021.

doi: <https://doi.org/10.1002/prot.26254>

[7] **Rahmatullah Roche**, Sutanu Bhattacharya, and Debswapna Bhattacharya. Hybridized distance- and contact-based hierarchical structure modeling for folding soluble and membrane proteins. *PLOS Computational Biology*, 2021.

doi: <https://doi.org/10.1371/journal.pcbi.1008753>

[8] Sutanu Bhattacharya, **Rahmatullah Roche**, Md Hossain Shuvo, and Debswapna Bhattacharya. Recent Advances in Protein Homology Detection Propelled by Inter-Residue Interaction Map Threading. *Frontiers in Molecular Biosciences*, 2021.

doi: <https://doi.org/10.3389/fmolb.2021.643752>

[9] Andrew J. McGehee, Sutanu Bhattacharya, **Rahmatullah Roche**, and Debswapna Bhattacharya. PolyFold: an interactive visual simulator for distance-based protein folding. *Plos One*, 2020.

doi: <https://doi.org/10.1371/journal.pone.0243331>

POSTERS AND PRESENTATIONS

Rahmatullah Roche, Sutanu Bhattacharya, and Debswapna Bhattacharya. Folding soluble and membrane proteins via hybridized distance and contact-based hierarchical structure modeling. (Highlight Talk) *ACM Bioinformatics Computational Biology*, 2021.

Sutanu Bhattacharya, **Rahmatullah Roche**, and Debswapna Bhattacharya. DisCover: distance- and orientation-based covariational threading for weakly homologous proteins
29th ISMB/ECCB conference, 2021.

Andrew McGehee, Sutanu Bhattacharya, **Rahmatullah Roche**, and Debswapna Bhattacharya. PolyFold: an interactive visual simulator for distance-based protein folding.
ACM Bioinformatics Computational Biology, 2020.

ABSTRACTS

Rahmatullah Roche, Sutanu Bhattacharya, and Debswapna Bhattacharya. Hybridized distance- and contact-based hierarchical protein structure modeling using DConStruct.

Proceedings of the 12th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics, 2021.

doi: <https://doi.org/10.1145/3459930.3469491>

Md Hossain Shuvo , Sutanu Bhattacharya , **Rahmatullah Roche** , and Debswapna Bhattacharya. Protein tertiary structure prediction by Bhattacharya group in CASP14. *CASP14 Abstract*, 2020.

https://predictioncenter.org/casp14/doc/CASP14_Abstracts.pdf

AWARDS

Pratt Fellowship Award 2023
Virginia Tech

Best Poster Award for 'PolyFold' 2020
ACM Bioinformatics and Computational Biology

Graduate school tuition fellowship 2018-2021
Auburn University

PUBLICLY AVAILABLE SCIENTIFIC SOFTWARE DEVELOPMENT

EquiPPIS Protein-protein interaction site prediction	2023
PIQLE Protein-protein interface quality estimation method	2023
rrQNet Protein contact map quality estimation	2022
DConStruct Hybridized distance- and contact-based hierarchical protein folding	2021
DisCovER Distance- and orientation-based Covariational threadER	2021

COMMUNITY INVOLVEMENT

Volunteered Engineering Day (E-day) Samuel Ginn College of Engineering	2019, 2020 Auburn, AL
Judged Poster Presentation Auburn Research Student Symposium	2019 Auburn, AL

SKILLS

Data Science/ML tools: PyTorch, TensorFlow, R
Programming Languages: C, C++, Java, Python
Molecular Visualization: Chimera, PyMOL
Database: Oracle, MySQL
Scripting: Linux Shell Script, LaTeX, HTML
Server Side Scripting: PHP

RESEARCH PROJECTS

Computational Protein Folding and Interactions Working on protein folding problem under the supervision of Dr. Debswapna Bhattacharya, Dept of CS, Virginia Tech. I have extensive experience in utilizing optimization algorithms to predict three-dimensional protein structures utilizing inter-residue interactions. Moreover, I am actively working on developing novel methods for predicting both intra- and inter-molecular interactions, including protein-protein and protein-nucleic acid interactions, by leveraging deep learning techniques.	Ongoing
Scheduler Worked on solving scheduling problems under the supervision of Dr. Abu Wasif, Dept of CSE, BUET. Two famous research scheduling problems (Vehicle Routing and Nurse Scheduling Problem) was approximately solved in feasible time, using different approaches: Genetic Algorithm, Local Search and Harmony Search Algorithm, and their hybridization. Developed tool that helps users visualize and taking decisions in any kind of employee scheduling, and route scheduling problem.	2015