

Md Hossain Shuvo, Ph.D.

Assistant Professor

Department of Computer Science
Prairie View A&M University
Prairie View, TX USA

Email: mhshuvo@pvamu.edu
Phone: (936) 261 9878
Web: <https://mdhossainshuvo.github.io>

EDUCATION

DEC 2023	Virginia Tech Ph.D. in Computer Science Advisor: Dr. Debswapan Bhattacharya GPA: 3.88/4.0
JUL 2017	Alabama A&M University M.Sc. in Computer Science Advisor: Dr. Yujian Fu GPA: 4.0/4.0
JUL 2014	Bangladesh University of Business and Technology B.Sc. in Computer Science Advisor: Mr. Md Saifur Rahman CGPA: 3.86/4.0

RESEARCH INTERESTS

Computational Biology
Machine Learning
Data Analytics
Artificial Intelligence

RESEARCH EXPERIENCE

AUG 2021 – DEC 2023	Virginia Tech Advisor: Dr. Debswapan Bhattacharya Research direction: application of machine learning in developing computational methods for addressing problems related to protein complexes
JAN 2018 – JUL 2021	Auburn University Advisor: Dr. Debswapan Bhattacharya

AUG 2015 – JUL 2017	Research direction: application of machine learning in developing computational methods for addressing problems related to protein structure prediction
	Alabama A&M University Advisor: Dr. Yujian Fu Research direction: development of tools for analyzing interactive behaviors in embedded and heterogeneous robotic systems

ACADEMIC EXPERIENCE

JAN 2024 - PRESENT	Prairie View A&M University Position: Assistant Professor, Dept. of CS
AUG 2018 – JAN 2020	Auburn University Position: Graduate Teaching Assistant, Dept of CSSE Courses: 1. COMP 5970/6970: Computational Biology 2. COMP1210: Fundamental of Computing I
MAY 2016 – JUL 2016	North Alabama Center for Educational Excellence (NACEE) Position: Assistant Mentor Topic: implementing multi-tasking and interactive behavior in NAO Humanoid robot
JAN 2015 – JUL 2015	Dhaka Commerce College, Dhaka, Bangladesh Position: Lecturer, Dept. of Stat, Math and COMP
JAN 2014 – DEC 2014	Dhaka Cambrian College, Dhaka, Bangladesh Position: Lecturer, Dept. of Information and Communication Technology

REFEREED PUBLICATIONS

2025

18. **M. H. Shuvo**, D. Bhattacharya. EquiRank: improved protein-protein interface quality estimation using protein-language-model-informed equivariant graph neural networks International Conference on Intelligent Biology and Medicine, 2024 Computational and Structural Biotechnology Journal, Volume 27, 160 - 170, 2025

2024

17. R. Roche, B. Moussad, **M. H. Shuvo**, S. Tarafder, D. Bhattacharya, EquiPNAS: improved protein-nucleic acid binding site prediction using protein-language-model-informed equivariant deep graph neural networks. *Nucleic Acids Research*, 2024 gkae039, 10.1093/nar/gkae039

2023

16. **M. H. Shuvo**, M. Karim, R. Roche, and D. Bhattacharya, “PIQLE: protein-protein interface quality estimation by deep graph learning of multimeric interaction geometries”, Bioinformatics Advances, 2023, vbad070, 10.1093/bioadv070.
15. **M. H. Shuvo**, M. Karim, and D. Bhattacharya, “iQDeep: an integrated web server for protein scoring using multiscale deep learning models”, Journal of Molecular Biology, 168057, 2023. doi: 10.1016/j.jmb.2023.168057
14. R. Roche, B. Moussad, **M. H. Shuvo**, D. Bhattacharya, “E(3) equivariant graph neural networks for robust and accurate protein–protein interaction site prediction”, PLOS Computational Biology, 19, e1011435, doi: 10.1371/journal.pcbi.1011435
13. S. Bhattacharya, R. Roche, **M. H. Shuvo**, and D. Bhattacharya, “Contact-assisted threading in low-homology protein modeling”, Methods in Molecular Biology book series, vol. 2627, 2023, doi: 10.1007/978-1-0716-2974-1_3

2022

12. R. Roche, S. Bhattacharya, **M. H. Shuvo**, and D. Bhattacharya, “rrQNet: Protein contact map quality estimation by deep evolutionary reconciliation”, Proteins, Jun 2022, doi: 10.1002/prot.26394.

2021

11. **M. H. Shuvo**, M. Gulfam, and D. Bhattacharya, “DeepRefiner: high-accuracy protein structure refinement by deep network calibration”, Nucleic Acids Research, vol. 49, no. W1, pp. W147–W152, Jul. 2021, doi: 10.1093/nar/gkab361
10. S. Bhattacharya, R. Roche, **M. H. Shuvo**, and D. Bhattacharya, “Recent Advances in Protein Homology Detection Propelled by Inter-Residue Interaction Map Threading”, Front Mol Biosci, vol. 8, p. 643752, 2021, doi: 10.3389/fmolb.2021.643752.
9. A. Kryshtafovych, . . . , **M. H. Shuvo**, . . . , “Modeling SARS-CoV-2 proteins in the CASP-commons experiment”, Proteins, vol. 89, no. 12, pp. 1987–1996, Dec. 2021, doi: 10.1002/prot.26231.

2020

8. **M. H. Shuvo**, S. Bhattacharya, and D. Bhattacharya, “QDeep: distance-based protein model quality estimation by residue-level ensemble error classifications using stacked deep residual neural networks”, Bioinformatics, vol. 36, no. Suppl 1, pp. i285–i291, Jul. 2020, doi: 10.1093/bioinformatics/btaa455
7. R. Alapati, **M. H. Shuvo**, and D. Bhattacharya, “SPECS: Integration of side-chain orientation and global distance-based measures for improved evaluation of protein structural models”, PLoS One, vol. 15, no. 2, p. e0228245, 2020, doi: 10.1371/journal.pone.0228245

2016

6. **M.H. Shubo**, Y. Fu, “Sonar sensor virtualization for object detection and localization”, SoutheastCon 2016, 1–8. doi: 10.1109/SECON.2016.7506699
5. Y. Fu, **M.H. Shubo**, “An approach to analyzing adaptive intelligent vehicle system using SMT solver”, In 2016 International Conference on Control, Decision and Information Technologies”, (CoDIT), pp. 313–319, doi: 10.1109/CoDIT.2016.7593580
4. Y. Fu, **M.H. Shubo**, “Android-Based Remote Robot Control System”. In, 2016 ASEE Annual Conference & Exposition Proceedings. ASEE Conferences, New Orleans, Louisiana, p.26251, doi: 10.18260/p.26251

2015

3. S. Rahman, **M.H. Shuvo**, "Advancement of Information System in the Health Sphere in Rural-Urban Areas of Developing Countries: A Case Study of Bangladesh". IJIRSET, Vol. 4, Issue 6, June 2015, doi: 10.15680/IJIRSET.2015.0406131
2. **M.H. Shuvo**, T. Haque, "Suspicious Behavior Detection Framework for Social Networking Sites Using Hidden Markov Model", 2015 Dhaka Commerce College Journal, Vol 7, Issue 1, P. 173 – 192

2014

1. M.M. Rahman, S. Ahmed, **M.H. Shuvo**, "Nearest Neighbor Classifier Method for Making Loan Decision in Commercial Bank". IJISA, 6, 60–68, doi: 10.5815/ijisa.2014.08.07

ABSTRACTS AND POSTERS

Abstracts

9. **M. H. Shuvo**, M. Karim, and D. Bhattacharya, "Protein modeling and accuracy estimation by Bhattacharya group in CASP15," CASP15 abstract, p. 35, 2022.
8. **M. H. Shuvo**, M. Gulfam, and D. Bhattacharya, "Deep network calibration for protein structure refinement," 13th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics, ACM-BCB 2022.
7. **M. H. Shuvo**, S. Bhattacharya, R. Roche, and D. Bhattacharya, "Protein tertiary structure prediction by Bhattacharya group in CASP14," CASP14 abstract, p. 38, 2020.
6. **M. H. Shuvo**, and D. Bhattacharya, "Protein model accuracy estimation by Bhattacharya groups in CASP14," CASP14 abstract, p. 39, 2020.
5. **M. H. Shuvo**, and D. Bhattacharya, "Protein structure refinement by Bhattacharya groups in CASP14," CASP14 abstract, pp. 40–41, 2020.
4. D. Bhattacharya, R. Alapati, and **M. H. Shuvo**, "Protein structure prediction and refinement by Bhattacharya human group in CASP13," CASP13 abstract, pp. 29-30, 2018.
3. R. Alapati, **M. H. Shuvo**, and D. Bhattacharya, "clustQ: Multi-model QA using superposition-free weighted internal distance comparisons," CASP13 abstract, p. 31, 2018
2. D. Bhattacharya and **M. H. Shuvo**, "refineD: Protein structure refinement using machine learning guided restrained relaxation," CASP13 abstract, p. 32, 2018
1. D. Bhattacharya and **M. H. Shuvo**, "scoreD: Estimating Global Distance Test using deep discriminative binary classifier ensemble," CASP13 abstract, p. 33

Posters

3. **M. H. Shuvo**, D. Bhattacharya. "EquiRank: improved protein-protein interface quality estimation using protein-language-model-informed equivariant graph neural networks", PVAMU R&I Week, 2024
2. S. Adepoju, **M.H. Shubo**, "How Machine Learning Can Revolutionize Building Comfort: Unveiling the Impact of Occupancy Prediction Models on HVAC Control System of the Roy G. Perry College of Engineering Building", PVAMU R&I Week, 2024
1. **M. H. Shubo**, S. Bhattacharya, D. Bhattacharya, "QDeep: distance-based protein model quality estimation by residue-level ensemble error classifications using stacked deep residual neural networks", ISMB 2020

Talks and Presentations

#	Year	Description
9	2025	Presented research works at the CCSB seminar titled “Data-Driven AI Frameworks toward Computational Drug Discovery”
8	2025	Presented a research work at the CCSB seminar titled “Toward reliability evaluation of computational models of protein molecules and their interactions”
7	2024	Presented research work on Faculty Research Day at PVAMU R&I Week titled “EquiRank: improved protein complex quality estimation with protein-language-model-informed Equivariant Graph Neural Network (EGNN)”
6	2024	Presented an invited talk in the Department of Computer Science titled “Quality Estimation of Computational Protein Models Using Machine Learning”
5	2024	Presented a research paper at the ICIBM 2024 conference titled “EquiRank: improved protein-protein interface quality estimation using protein-language-model-informed equivariant graph neural networks”
4	2022	Presented research article at MCBIOS 2022 conference titled “DeepRefiner: high-accuracy protein structure refinement by deep network calibration”
3	2020	Presented a poster at ISMB 2020 conference titled “QDeep: distance-based protein model quality estimation by residue-level ensemble error classifications using stacked deep residual neural networks”
2	2016	Presented a conference paper at IEEE SoutheastCon 2016 titled “Sonar sensor virtualization for object detection and localization”
1	2016	Presented a research poster at AAMU STEM Day 2016 titled “Collision Free Intelligent Parking System”

PARTICIPATION IN COMMUNITY-WIDE ASSESSMENT

APR 2022 – AUG 2022	15th Critical Assessment of Protein Structure Prediction (CASP15) challenge Role: method development, technical support for double-blind testing of our developed methods in both server and human pipelines
MAY 2020 – SEP 2020	14th Critical Assessment of Protein Structure Prediction (CASP14) challenge Role: method development, technical support for double-blind testing of our developed methods in both server and human pipelines
APR 2020	CASP Commons (COVID-19, 2020), a collaborative initiative for modeling the SARS-2-CoV structure Role: Provided technical support for testing our developed methods in predicting and assessing SARS-2-CoV target
MAY 2018 – AUG 2018	13th Critical Assessment of Protein Structure Prediction (CASP13) challenge

Role: method development, technical support for double-blind testing of our developed methods in both server and human pipelines

HONORS AND AWARDS

Quantum Workshop Travel Fellowship	By the University of Tennessee at Chattanooga
Google Cloud Research Resource	\$5,000 resource credit by Google
The PHIT Workforce Development Program Grant [Co-PI]	\$432,078 by the University of Texas Health Science Center at Houston
GenAI Faculty Summit Travel Fellowship	Awarded by Google
FACULTY ENHANCEMENT PROGRAM	Awarded by the Roy G. Perry College of Engineering at PVAMU
NSF NDSA PFx instructor	Selected to be a PFx instructor
NSF NDSA RESEARCH AFFINITY COHORT	Selected as 1 of the 20 researchers
GOOGLE TEC EQUITY IMPACT FUND	\$50,000 non-dilutive funding, led jointly with Dr. Wang at PVAMU
ACCESS ALLOCATIONS	Principal Investigator (PI), NSF - XSEDE Research Allocation
PRATT FELLOWSHIP AWARD	Awarded Pratt Fellowship at Virginia Tech, 2023
YOUNG SCIENTIST EXCELLENCE AWARDS	Awarded 1 st place prize at 18 th annual MCBIOS conference, 2022
CONFERENCE FELLOWSHIP	I. Received fellowship award for MCBIOS 2022 II. Received ISMB 2020 fellowship award
PUBLICATION RECOGNITION	DeepRefiner paper accepted for ACM-BCB 2022 Highlights track
TRAVEL FELLOWSHIP	Received travel grant for IEEE SoutheastCon 2016
POSTER AWARD	Awarded 2 nd place prize at AAMU STEM Day 2016

SCIENTIFIC SOFTWARE DEVELOPMENT

EquiRank	PLM-based Protein-protein interface quality estimation method [GitHub]
PIQLE	Protein-protein interface quality estimation method [GitHub]
iQDeep	Integrated protein scoring server [Server]
DeepRefiner	High-accuracy protein structure refinement server [Server]
QDeep	Single-model protein quality estimation method [GitHub]
SPECS	Improved evaluation method for protein structures [Github]
EquiPPIS	E(3) equivariant graph neural networks for robust and accurate protein-protein interaction site prediction [Github]

EquiPNAS	EquiPNAS: improved protein-nucleic acid binding site prediction using protein-language-model-informed equivariant deep graph neural networks [GitHub]
rrQNet	Protein contact map evaluation method [Github]

TECHNICAL SKILLS

PROGRAMMING SKILLS	Python, R, Java, C, C++, PHP, ASP, Apache Cordova MySQL, MSSQL
APP DEVELOPMENT	<ul style="list-style-type: none"> I. Predictive applications using Machine Learning II. Standalone application development with Java EE III. Mobile applications development in both Android and iOS IV. Platforms Web applications development V. Robotic applications development for EV3, NAO, and UAV

SERVICES AND OUTREACH

FACULTY ADVISORY COUNCIL	Serving as a member of the Faculty Advisory Council for the College of Engineering at PVAMU
COMPUTER SCIENCE CURRICULUM DEVELOPMENT COMMITTEE	Serving as a member of the CS Undergraduate Curriculum Development Committee
COLLEGE OF ENGINEERING CURRICULUM DEVELOPMENT COMMITTEE	Served as a member of the COE Undergraduate Curriculum Development Committee
DIVISION OF RESEARCH AND INNOVATION COMMITTEE	Serving as a member of the Division of Research and Innovation Committee for Computer Science at PVAMU
FACULTY SEARCH COMMITTEE	Served as a member of the PVAMU faculty search committee
REVIEWER	Served as a sub-reviewer for Bioinformatics, ISMB, BIOKDD, CAMD, IEEE ACM/Transaction/CogMI, and others
EVENT MANAGEMENT	<ul style="list-style-type: none"> i. Provided logistic support on E-day 2020 at Auburn University ii. Provided logistic support on AAMU Senior High School Day 2016
TECHNICAL COMMITTEE MEMBER	Provided technical support by developing the complete submission management system for AAMU STEM Day 2016