Md Hossain Shuvo, Ph.D. Assistant Professor

Department of Computer Science	Email: <u>mhshuvo@pvamu.edu</u>
Prairie View A&M University	Phone: (936) 261 9878
Prairie View, TX USA	Web: https://mdhossainshuvo.github.io

EDUCATION

DEC 2023	Virginia Tech
	Ph.D. in Computer Science
	Advisor: Dr. Debswapna 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. Debswapna 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. Debswapna Bhattacharya

	Research direction: application of machine learning in developing computational methods for addressing problems related to protein structure prediction
AUG 2015 – JUL 2017	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:
	 COMP 5970/6970: Computational Biology 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

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.
- 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

- 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.
- A. Kryshtafovych, . . . , M. H. Shuvo, . . . , "Modeling SARS-CoV-2 proteins in the CASPcommons experiment", Proteins, vol. 89, no. 12, pp. 1987–1996, Dec. 2021, doi: 10.1002/prot.26231.

2020

- 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
- 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. Shuvo**, Y. Fu, "Sonar sensor virtualization for object detection and localization", SoutheastCon 2016, 1–8. doi: 10.1109/SECON.2016.7506699
- Y. Fu, M.H. Shuvo, "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. Shuvo**, "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
- 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

 M. H. Shuvo, 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

PARTICIPATION IN COMMUNITY-WIDE ASSESSMENT

APR 2022 – AUG 2022	15 th 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	14 th 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

13th Critical Assessment of Protein Structure Prediction MAY 2018 – AUG 2018 (CASP13) challenge **Role:** method development, technical support for double-blind

testing of our developed methods in both server and human pipelines

HONORS AND AWARDS

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	 Received fellowship award for MCBIOS 2022 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

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

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PROGRAMMING SKILLS	Python, Java, C, C++, PHP, ASP, Apache Cordova MySQL, MSSQL
APP DEVELOPMENT	 I. Standalone application development with Java EE II. Mobile applications development in both Android and iOS

III. Platforms Web applications development IV. Robotic applications development for EV3, NAO, and UAV

SERVICES AND OUTREACH

REVIEWER	Served as a sub-reviewer for BIOKDD 2021, 2023
EVENT MANAGEMENT	 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