Md Hossain Shuvo
Ph.D. Candidate

Department of Computer Science
Virginia Tech
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EDUCATION

AUG 2021 - PRESENT — **Virginia Tech**
Ph.D. candidate in Computer Science
Advisor: Dr. Debswapna Bhattacharya
GPA: 3.88/4.0

JAN 2018 - JUL 2021 — **Auburn University**
Ph.D. student in Computer Science and Software Engineering (Transfer Out)
Advisor: Dr. Debswapna Bhattacharya
GPA: 3.92/4.0

AUG 2015 - JUL 2017 — **Alabama A&M University**
M.S. in Computer Science
Advisor: Dr. Yujian Fu
GPA: 4.0/4.0

MAY 2010 - JUL 2014 — **Bangladesh University of Business and Technology**
B.S. in Computer Science
Advisor: Mr. Md. Saifur Rahman
CGPA: 3.86/4.0

RESEARCH INTERESTS

Computational Biology
Applied Machine Learning
Data Science in Bioinformatics

RESEARCH EXPERIENCE

AUG 2021 – PRESENT — **Virginia Tech**
Advisor: Dr. Debswapna Bhattacharya
Research direction: Application of machine learning in developing 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 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 embedded and heterogeneous robotic systems.

REFEREED PUBLICATIONS

1. **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
2. **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.
3. **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.
4. **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.
5. 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.
6. 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.
7. 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. bioRxiv, 2023.09.14.557719.
8. 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.
10. 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.
11. 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

ABSTRACTS AND POSTERS

ABSTRACTS

1. **M. H. Shuvo**, M. Karim, and D. Bhattacharya, "Protein modeling and accuracy estimation by Bhattacharya group in CASP15," CASP15 abstract, p. 35, 2022.
2. **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.
3. **M. H. Shuvo**, S. Bhattacharya, R. Roche, and D. Bhattacharya, "Protein tertiary structure prediction by Bhattacharya group in CASP14," CASP14 abstract, p. 38, 2020.
4. **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.
6. 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.
7. R. Alapati, **M. H. Shuvo**, and D. Bhattacharya, "clustQ: Multi-model QA using superposition-free weighted internal distance comparisons," CASP13 abstract, p. 31, 2018.
8. D. Bhattacharya and **M. H. Shuvo**, "refineD: Protein structure refinement using machine learning guided restrained relaxation," CASP13 abstract, p. 32, 2018.
9. D. Bhattacharya and **M. H. Shuvo**, "scoreD: Estimating Global Distance Test using deep discriminative binary classifier ensemble," CASP13 abstract, p. 33.

POSTERS

1. **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.

TEACHING EXPERIENCE

AUG 2018 – JAN 2020 — **Auburn University**

Position: Graduate Teaching Assistant, Dept. of CSSE

Courses:

i. COMP 5970/6970: Computational Biology
ii. COMP1210: Fundamental of Computing I

AUG 2016 - JUL 2017 — **Alabama A&M University**

Position: Graduate Teaching Assistant, Dept. of Computer Science

Courses:

i. CS 102: Introduction to Programming
ii. EGC 104: Computer Programming

MAY 2016 - JUL 2016 — **North Alabama Center for Educational Excellence (NACEE)**

Position: Assistant Mentor

Topic: Implementing Multitasking and Interactive Behavior in NAO Humanoid Robot.

JAN 2015 - JUL 2015 — **Dhaka Commerce College, Dhaka, Bangladesh**

	Position: Lecturer, Dept. of Statistics, Mathematics, and Computer
JAN 2014 - DEC 2014	**Dhaka Cambrian College, Dhaka, Bangladesh** **Position:** Lecturer, Dept. of Information and Communication Technology

PARTICIPATION IN COMMUNITY-WIDE ASSESSMENT

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

HONORS AND AWARDS

PRATT FELLOWSHIP AWARD	Awarded Pratt Fellowship at Virginia Tech, 2023.
YOUNG SCIENTIST EXCELLENCE AWARDS	Awarded 1st place prize at 18th 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 the ACM-BCB 2022 Highlights Track
TRAVEL FELLOWSHIP	Received travel grant for IEEE SoutheastCon 2016
POSTER AWARD	Awarded 2nd 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]
EquiPNAS	EquiPNAS: improved protein-nucleic acid binding site prediction using protein-language-model-informed equivariant deep graph neural networks [GitHub]
EquiPPIS	E(3) equivariant graph neural networks for robust and accurate protein–protein interaction site prediction [GitHub]
rrQNet	Protein contact map evaluation method [GitHub]

TECHNICAL SKILLS

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 Platforms iii. 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

AFFILIATIONS

1. International Society for Computational Biology (ISCB)