Kevin Molloy September 2023
Assistant Professor molloykp@jmu.edu
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Education

- **George Mason University** Fairfax, VA
  Ph.D. Computer Science *2011 – 2015*
  - Dissertation Title: Probabilistic Algorithms for Modeling Protein Structure and Dynamics
  - Dissertation Advisor: Amarda Shehu
  - Research Interests: Computational Biology, Robotic Motion Planning, Machine Learning
  - Graduate Research Assistant in Shehu Computational Biology Lab
- **George Mason University** Fairfax, VA
  M.S. Computer Science *2008 – 2011*
  - Advisor: Amarda Shehu
  - Thesis: “Variable-Length Fragment Assembly within a Probabilistic Protein Structure Prediction Framework” defended in Summer 2011 (Committee details here).
  - Outstanding Academic Achievement Award (3.96 GPA)
- **George Mason University** Fairfax, VA
  B.S. Computer Science *1989 – 1998*

Employment

- **James Madison University** Harrisonburg, VA, USA
  Assistant Professor Computer Science Department *August 2018 - current*
  Affiliate Appointment, Department of Biology *May 2019 - current*
- **George Mason University** Fairfax, VA, USA
  Visiting Researcher and Adjunct Professor Computer Science Department *August 2016 - May 2018*
- **Centre National de la recherche Scientifique** Toulouse, France
  Postdoctoral Researcher *March 2015 - August 2016*
- **George Mason University** Fairfax, VA, USA
  Graduate Research Assistant *May 2012- January 2015*
- **George Mason University** Fairfax, VA, USA
  Graduate Teaching Assistant *Aug 2011- May 2012*
- **Molloy Software Associates, Inc.** Centreville, VA, USA
  Database Architect *Feb 1997 - Aug 2018*

Research

My research focuses on the development of algorithms to study complex systems and their characteristics. My work in structure biology is aimed at developing algorithms to unravel the relationship between protein sequence, protein structure, and protein motion/dynamics. My current work focuses on small flexible regions of proteins known as loops and small peptides known as AMPs (antimicrobial peptides). AMPs are an important component in the effort to combat antibiotic resistant bacteria. Additionally work involves computationally identifying variants of the SARS-2-COV virus which exhibit structural modifications that result in different behavior and interactions with antibodies. My other research interests include robot motion planning, machine learning/pattern recognition, and artificial intelligence.

Awards

College of Integrated Science and Engineering Junior Faculty Award	February 2023
Davies-Yaskins Faculty Support Endowment	January 2020
George Mason University Computer Science Outstanding Graduate Student Award	May 2015
Nominee for best paper award for BiCoB conference	March 2014
ACM Recognition of Service Award (Conference Volunteer for ACM-BCB)	September 2013
Dean Fellowship	2011 – 2012
Outstanding Academic Achievement M.S. Computer Science	2008 – 2011
Best student paper award BIONETICS conference	December 2010

Publications

Journal Articles (peer-reviewed)

13. A. Barozet, K. Molloy, M. Vaisset, C. Zanon, P. Fauret, Thierry Siméon, J. Cortés. MoMA-LoopSampler: A web server to exhaustively sample protein loop conformations. *Oxford Bioinformatics*, Vol. 38, Issue 2, pages 552-553, January 2022. [IF: 5.6] [Citations: 2].

12. A. Barozet, K. Molloy, M. Vaisset, Thierry Siméon, J. Cortés. A Reinforcement Learning Approach to Enhance Exhaustive Protein Loop Sampling. *BMC Bioinformatics*, Vol. 36, Issue 4, pages 1099-1106, February 2020. [IF: 5.6] [Citations: 20].

11. A. Estaña, K. Molloy, M. Vaisset, B. Sibille, T. Siméon, P. Bernadó, J. Cortés. Hybrid parallelization of a multi-tree path search algorithm: Application to highly-flexible biomolecules. Parallel Computing, Vol 77 June 2018 [IF: 1.36] [Citations: 12]

10. Kevin Molloy, Laurent Denarie, Marc Vaisset, Thierry Siméon, and Juan Cortés. Simultaneous System Design and Path Planning. Intl. Journal of Robotics Research (IJRR), July 2018. [IF: 2.50] [Citations: 15]

9. Kevin Molloy, Amarda Shehu. A General, Adaptive, Roadmap-based Algorithm for Protein Motion Computation. IEEE Trans NanoBioScience (TNB) 15(2): 158-165. March 2016. [IF: 1.77] [Citations: 18]

8. Didier Devaurs, Kevin Molloy, Marc Vaisset, Amarda Shehu, Thierry Siméon, and Juan Cortés. Characterizing Energy Landscapes of Peptides using a Combination of Stochastic Algorithms. IEEE Trans NanoBioScience, 2015, 14:545-552. [IF: 1.77] [Citations: 31]

7. Kevin Molloy, Rudy Clausen, Amarda Shehu. A Stochastic Roadmap Method to Model Protein Structural Transitions. *Robotica*, December 2015. [IF: 0.894] [Citations: 14]. (Featured on journal cover)

6. Kevin Molloy, M. Jennifer Van, Daniel Barbará and Amarda Shehu. Exploring representations of protein structure for automated remote homology detection and mapping of protein structure space. *BMC Bioinformatics*, 15 (Suppl 8):S4, 2014. [IF: 3.02] [Citations: 13]

5. Kevin Molloy, Sameh Saleh, and Amarda Shehu. Probabilistic Search and Energy Guidance for Biased Decoy Sampling in Ab-initio Protein Structure Prediction. *IEEE Transactions in Computational Biology and Bioinformatics*,10(5):1162-1175, 2013. [IF: 2.25] [Citations: 45]

4. Kevin Molloy and Amarda Shehu. Elucidating the Ensemble of Functionally-relevant Transitions in Protein Systems with a Robotics-inspired Method. *BMC Structural Biology Journal*, 13(Suppl 1):S8, 2013. [IF: 2.09] [Citations: 22]

3. Brian Olson, Irina Hashmi, Kevin Molloy, and Amarda Shehu. Basin Hopping as a General and Versatile Optimization Framework for the Characterizations of Biological Macromolecules. *Advances in Artificial Intelligence*, 2012, 674832. [Citations: 85]

2. Brian Olson, Kevin Molloy, S. Farid Hendi, Amarda Shehu. Guiding Search in the Protein Conformational Space with Structural Profiles. *Journal of Bioinformatics and Computational Biology*, 2012, 10(3):1242005. [IF: 1.06] [Citations: 27]

1. Brian Olson, Kevin Molloy, Amarda Shehu. In Search of the Protein Native State with a Probabilistic Sampling Approach. *Journal of Bioinformatics and Computational Biology*, 9(3):383-398. [IF: 1.06] [Citations: 37]

Book Chapters

2. Nurit Haspel, Filip Jagodzinski, Kevin Molloy (editors). Algorithms and Methods in Structural Bioinformatics, Springer, 2022.[Citations:1]

1. Amarda Shehu, Daniel Barbará, and Kevin Molloy. A Survey of Computational Methods for Protein Function Prediction. In Big Data Analytics in Genomics (Springer), first edition, (Editors: Wong, K. C.), 2016. [Citations: 69]

Conference Proceedings (peer-reviewed)

8. Thura, Sanda and Forsyth, Jason and Molloy, Kevin and Couch, Jacob. Analysis of the Machine Learning Classification of Cardiac Disease on Embedded Systems. 2023 Systems and Information Engineering Design Symposium (SIEDS), Charlottesville, VA. 2023.

7. Laurent Denarie, Kevin Molloy, Marc Vaisset, Thierry Siméon, and Juan Cortés. Combining System Design and Path Planning. International Workshop on the Algorithmic Foundations of Robotics(WAFR), San Francisco, CA, 2016. [Citations: 7]

6. Kevin Molloy and Amarda Shehu. Interleaving Global and Local Search for Protein Motion Computation. International Symposium on Bioinformatics Research and Applications (ISBRA), Norfolk, VA, 2015. [Citations: 11]

5. Kevin Molloy and Amarda Shehu. A Probabilistic Roadmap-based Method to Model Conformational Switching of a Protein Among Many Functionally-relevant Structures. *6th International Conf on Bioinformatics and Computational Biology (BiCOB)*, Las Vegas, NV, 2014 *(finalist for best paper award)*. [Citations: 2]

4. Kevin Molloy, Jennifer M. Van, Daniel Barbará, and Amarda Shehu. Higher-order Representations for Automated Organization of Protein Structure Space. *IEEE International Conf on Computational Advances in Bio and Medical Sciences (ICCABS)*, New Orleans, LA, 2013. [Citations: 1]

3. Kevin Molloy and Amarda Shehu. Biased Decoy Sampling to Identify Near-Native Protein Conformations. *ACM Bioinf. and Comp. Biology (BCB)*, Orlando FL 2012, pg. 131-138. [Citations: 7]

2. Brian Olson, Kevin Molloy, and Amarda Shehu. Enhancing Sampling of the Conformational Space Near the Protein Native State. In *Intl. Conf Bio-inspired Models of Network, Information, and Computing Systems (BIONETICS)*, LNICST (Springer), vol. 87, pg. 249-263, Boston, MA, 2010 *(best student paper award)*. [Citations: 15]

1. Kevin Molloy and Daniel Menascé. Method and Model to Assess the Performance of Clustered Databases: The Oracle RAC Case. In *Computer Measurement Group (CMG)* , Orlando, FL. December 2010. [Citation: 1]

Workshop Proceedings (peer-reviewed)

3. Darren McKnight, Kevin Molloy, Seth Speaks, Cullen O'Hara. Applying Machine Learning to Enhance Conjunction Prediction. Key Topics in Orbit Propagation Applied to Space Situational Awareness (kePASSA). La Rioja, Spain. April 2019.

2. Kevin Molloy, Rudy Clausen, and Amarda Shehu. On the Stochastic Roadmap to Model Functionally-related Structural Transitions in Wildtype and Varient Proteins. *Workshop on Robotics Methods for Structural and Dynamic Modeling of Molecular Systems*, Berkeley, California, July 2014.

1. Kevin Molloy and Amarda Shehu. A Robotics-inspired Method to Sample Conformational Paths Connecting Known Functionally-relevant Structures in Protein Systems. In *Comput Struct Biol Workshop (CSBW)*, IEEE BIBM Workshops, Philadelphia, PA, 2012, pg. 56-63. [Citations: 4]

Extended Abstracts and Posters

8. Dakota Scott, Sanda Thura, and Kevin Molloy. A Computational Pipeline to Detect Novel SARS-2-COV Variants. July 2022 at the Bio-Chem REU hosted at James Madison University.

7. Cameron Kelahan, Anca Constantin, Kevin Molloy. A Machine Learning Approach to Improve the Water Megamaser Detection Rates. *American Astronomical Society Meeting Abstracts*, vol. 53, June 2021.

6. Emma Macaluso, Kevin Molloy. Characterizing Antimicrobial Peptides with Computational Techniques. CAPWIC 2021.

5. Nathan Moore, Kevin Molloy, William Lovo, Sven Mayer, Pawel W. Wozniak, and Michael Stewart. POST: A Machine Learning Based Paper Organization and Scheduling Tool. *Proceedings of the 2020 ACM International Conference on Supporting Group Work*. Janurary 2020.

4. Kevin Molloy, Nicolas Buhours, Marc Vaisset, Thierry Siméon, Étienne Ferré and Juan Cortés. A Reinforcement Learning Approach to Protein Loop Modeling. *Machine Learning in Planning and Control of Robot Motion Workshop at IROS 2015*, Hamburg Germany, Oct 2015. [Citations: 2]

3. Kevin Molloy and Amarda Shehu. A tree-based search to bias sampling of protein decoy conformations. *IEEE BIBM*, pg. 978, Philadelphia, PA, October 4-7, 2012.

2. Kevin Molloy and Amarda Shehu. Mapping conformational pathways between known functional protein states. *CSBW at IEEE BIBM Workshops (BIBM-W)*, pg. 971, Philadelphia, PA, October 4-7, 2012.

1. Kevin Molloy and Amarda Shehu. Assembly of low-energy protein conformations with heterogeneous fragments. *IEEE BIBM*, pg. 991-993, Atlanta, GA, November 12-15, 2012.

Talks

17. Advances in Protein Characterizations. James Madison University Computer Science. March 2022.
16. Employing Deep Learning to Study Biomolecules. A tutorial presented at the ACM Bioinformatics and Computational Biology (BCB) in Niagara Falls, NY. Sept 2019.
15. Investigating Protein Structure, Function and Design with Robotics-inspired methods and Machine Learning. Seminar Series on Biology at James Madison University, Harrisonburg, VA. February 2019.
14. The intersection of Computer Science, Biology, and Robotics. Invited speaker at Hampton Road Academy, Newport News, Va. January 2019.
13. Modeling Macromolecular Structures and Motions. Computational Methods for Sampling and Analysis of Energy Landscapes. ACM-BCB (Bioinformatics, Computational Biology, and Health Informatics), Washington, DC. August 2018.
12. Applying Robotics and Machine Learning Methods to Investigate Protein Structure and Dynamics. Computer Science Department, James Madison University, March 2018.
11. Robotics-inspired Algorithms for Modeling Protein Structures and Motions. ACM-BCB (Bioinformatics, Computational Biology, and Health Informatics), Boston, MA. August 2017.
10. Combining System Design and Path Planning. International Workshop on the Algorithmic Foundations of Robotics (WAFR), San Francisco, California, December 2016.
9. Characterizing Energy Landscapes of Small Peptides. Atomic and Molecular Computation Workshop, University Paul Sabatier, Toulouse, France, November 2015.
8. Probabilistic Algorithms for Modeling Protein Structure and Dynamics, Robotics and Interactions research group. LAAS/CNRS, Toulouse, France, April 2015.
7. Probabilistic Algorithms for Modeling Protein Structure and Dynamics. Computational Materials Science Center and the School of Physics, Astronomy, & Computational Sciences. George Mason University, Fairfax, VA. February 2015.
6. Algorithmic Frameworks for Modeling Structures, Motions, and Assembly of Protein Mo;ecules. Guest lecturer for BENG 420 (Bioinformatics for Engineers), Volgenau School of Engineering (VSE), George Mason University, Fairfax, VA. October 2014.
5. On the Stochastic Roadmap to Model Functionally-related Structural Transitions in Wildtype and Variant Proteins. RSS Workshop on Robotics Methods for Structural and Dynamic Modeling of Molecular Systems (RMMS), Berkeley, CA, USA, July 2014.
4. Higher-order Representations for Automated Organization of Protein Structure Space. Intl Conf on Computational Advances in Bio and Medical Sciences (ICCABS), New Orleans, LA. June 2013.
3. A Robotics-inspired Method to Sample Conformational Paths Connecting Known Functionally-relevant Structures in Protein Systems. Computational Structure Biology Workshop (CSBW), Philadelphia, PA. Oct 2012.
2. Biased Decoy Sampling to Identify Near-Native Protein Conformations. ACM Bioinformatics and Computational Biology Conference (BCB), Orlando, FL. Oct. 2012.

1. Method and Model to Assess the Performance of Clustered Databases: The Oracle RAC Case. In *Computer Measurement Group (CMG)* , Orlando, FL. December 2010.

External Funding

3. **$40K** – Develop ensemble learning techniques for anomaly detection for use in identifying cyberattacks. Funding - VA CCI.
2. **$5K** – Characterizing Antimicrobial Peptides Utilizing Structure and Sequence Information. 4-VA Spring 2021.
1. **$17K** VIVA Course Redesign Grant for Open Access Undergraduate Robotics Textbook. PI - Nathan Sprague.

Teaching Experience

- **Introduction to Programming (CS 149)** James Madison University
  Assistant Professor *6 semesters including 2018(Fall) and 2021(Fall)*
- **Data Structures and Algorithms (CS 240)** James Madison University
  Assistant Professor *2022(Fall)*
- **Autonomous Robotics (CS 354)** James Madison University
  Assistant Professor *Fall 2020, Fall 2021*
- **Applied Algorithms (CS 412)** James Madison University
  Assistant Professor *Spring 2021, Spring 2022, Spring 2023, Fall 2023*
- **Artificial Intelligence (CS 444)** James Madison University
  Assistant Professor *Each Spring from 2019 to 2023*
- **Machine Learning (CS 445)** James Madison University
  Assistant Professor *Fall 2019, Fall 2020, Fall 2022, Fall 2023*
- **Principles of Computing (CS 100)** George Mason University
  Adjunct Professor *Fall 2017, Spring 2018*
- **Principles of Data Management and Mining (CS 504)** George Mason University
  Adjunct Professor *Fall 2016, Spring 2017, Fall 2017*
- **Software Engineering (CS 321)** George Mason University
  Graduate Teaching Assistant *Fall 2011 - Spring 2012*

Service

Current University and Department/College Committees

- JMU Honors College Liaison for the Computer Science Department (2023 - present)
- JMU Computer Science Theory/Algorithms Committee (2023 - present)
- JMU Fellowship Nomination Committee (2022 - present)
- JMU Robotics club faculty advisor (2022 - present)
- JMU CISE Faculty Leave and Grants Committee (Fall 2021/Spring 2022)
- JMU Computer Science First Year Advisor (2021 - present)
- JMU Computer Science Faculty Advisor (2021)
- JMU Computer Science Teaching Assistant Coordinator (2021 - present)
- JMU Computer Science PAC Junior Faculty Member(Fall 2021/Spring 2022)
- JMU Data Science 4 + 1 initiative (2018-2019)

Workshop Organization

- Co-chair for the "Computational Structural Bioinformatics Workshop". Sept 2020 in Atlanta, Georgia (but held virtually this year).
- Co-chair for the "Computational Structural Bioinformatics Workshop". August 2018 in Washington, DC.
- Co-chair for the "Computational Structural Bioinformatics Workshop". August 2017 in Boston, MA.
- Practical session organizer for "Algorithms in Structural Bioinformatics", December 2015 in Corsica, France.
- Student co-organizer for "Robotics Methods for Biological Structures and Kinematics Modeling" Workshop at RSS, July 16, 2014 Berkeley, CA.
- Local student volunteer at ACM BCB September 22-24, 2013 Washington, DC.

Student Advising and Mentoring

- Leonard Marsault – co-advised with Juan Cortés – undergraduate special project on Rapid Identification of Neighboring Protein Configurations

Masters Thesis Committee Member

- Committee Member, David Morris, *Snapshots and Springs: Analyzing and Reproducing the Motions of Molecules*, Computer Science (director: Amarda Shehu, committee Molloy K and Duric Z)

Undergraduate Honors Thesis Capstone

6. Sanda Thura. *Analysis of the Machine Learning Classification of Cardiac Disease on Embedded Systems.* Computer Science and Engineering, Spring 2023. Committee: Forsyth, J (directory), Molloy, K. (reader), Couch, J, (reader).
5. Endre Szakal. *Structural Fragment Libraries to Characterize Protein Structure*, Computer Science, Spring 2023. Committee: Molloy K (director), Bowers, J. (reader), Cresawn, Steven(reader)
4. Emma Macaluso, *Characterizing Antimicrobial Peptides with Computational Techniques*, Computer Science, Spring 2021. Committee: Molloy K (director), Weikle, D (reader), Wright, N (reader)
3. Sophie Marie Brause. *The Affect of Defensive Tactics on the Probability of a Pass being Successful in Soccer.* Spring 2021. Committee: Bernstein D (directory), Molloy K (reader), Weikle, D (reader)
2. William Lovo, *Detecting Credit Card Fraud: An Analysis of Fraud Detection Techniques*, Computer Science, Spring 2020. Committee: Molloy K (director), Sprague N (reader), Bowers J (reader), Lam, M (reader)
1. Anthony Snarr, *Towards Natural Language Understanding in Text-Based Games*, Computer Science, Spring 2020. Committee: Sprague N (director), Bernstein D (reader), Molloy K (reader)

Journal Referee

- IEEE/ACM Transactions on Computational Biology and Bioinformatics (TCBB)
- Proteome Science
- Journal of Chemical Information and Modeling
- IEEE Robotics and Automation Letters
- Biomolecules

Conference/Workshop Referee

- ACM Bioinf and Comp Biol (BCB), 2014, 2017, 2018, 2019
- CSBW - 2014, 2016, 2017, 2018, 2019, 2020, 2021, 2022, 2023
- IROS (Motion Planning), 2016
- WAFR (Robotics), 2016