

Kevin Molloy

Postdoctoral Fellow at LAAS/CNRS
Toulouse, France

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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

- **Centre National de la recherche Scientifique** Toulouse, France
Postdoctoral Researcher March 2015 - current
- **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 - current

Research

My research focus is on the development of algorithms to unravel the relationship between protein sequence, protein structure, and protein motion/dynamics. My research interests include protein modeling and design, bioinformatics, robot motion planning, machine learning/pattern recognition, and artificial intelligence. I am currently working as a postdoctoral fellow at CNRS in Toulouse France focusing on the development of novel algorithms for the optimization and de-novo design of proteins to modify and/or enhance their biological function.

Awards

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)

9. Kevin Molloy, Amarda Shehu. A General, Adaptive, Roadmap-based Algorithm for Protein Motion Computation. *IEEE Trans NanoBioScience* 2015 (in press). [IF: 1.77]
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]
7. Kevin Molloy, Rudy Clausen, Amarda Shehu. A Stochastic Roadmap Method to Model Protein Structural Transitions. *Robotica*, December 2015. [IF: 0.894]
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: 2]
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: 8]
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: 8]
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: 12]
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: 17]
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: 26]

Conference Proceedings (peer-reviewed)

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.
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: 1]
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 (ICCBS)*, 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: 6]

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: 14]
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.

Workshop Proceedings (peer-reviewed)

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

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 (extended abstract and poster).
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 (extended abstract and poster).
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 (extended abstract and poster).
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 (extended abstract and poster).

Talks

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 Molecules. 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 (ICCBMS), 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.

Teaching Experience

- **Software Engineering (CS 321)** George Mason University
Graduate Teaching Assistant *Fall 2011 - Spring 2012*
 – Grade homework assignments and assist students with writing assignments.

Service

Workshop Organization

- 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.

Journal Referee

- Proteome Science
- Journal of Chemical Information and Modeling

Conference Referee

- ACM Bioinf and Comp Biol (BCB), 2014