Mark Moll

moll.ai mark@moll.ai /mmoll /mamoll

Employment

Principal Research Scientist 11/2024–present
Senior Research Scientist 6/2023–11/2024
Metron, *Portland, OR*

Director of Research 9/2019–5/2023
PickNik Robotics, *Boulder, CO*

Senior Research Scientist 7/2016–11/2021
Adjunct Faculty Member 7/2011–11/2021
Research Scientist 3/2007–6/2016
Rice University, Department of Computer Science, *Houston, TX*

Computer Scientist 9/2005–2/2007
Polymorphic Robotics Lab, Information Sciences Institute, USC, *Marina del Rey, CA*

Postdoctoral Researcher 8/2002–8/2005
Rice University, Department of Computer Science and W.M. Keck Center for Comp. Bio., *Houston, TX*

Research Assistant 9/1996–7/2002
Manipulation Lab, Carnegie Mellon University, *Pittsburgh, PA*

Visiting Researcher 5/2001–8/2001
Berkeley Automation Sciences Lab, University of California at Berkeley, *Berkeley, CA*

Researcher 9/1995–8/1996
Centre for Science and Technology Studies, Leiden University, *Leiden, The Netherlands*

Research Assistant 1/1995–8/1995
Parlevink Language Engineering Group, University of Twente, *Enschede, The Netherlands*

Visiting Researcher 9/1993–12/1993
Neural Nets Research Group, University of Texas, *Austin, TX*

Education

Carnegie Mellon University, *Pittsburgh, PA* 9/1996–8/2002
Ph.D. in Computer Science
Thesis title: Shape Reconstruction Using Active Tactile Sensors
Thesis advisor: Professor Michael A. Erdmann

University of Twente, *Enschede, The Netherlands* 9/1990–8/1995
M.S. in Computer Science
Thesis title: Head-Corner Parsing Using Typed Feature Structures
Thesis advisor: Dr. Rieks op den Akker

Further Education

Deep Learning Specialization, *deeplearning.ai, Coursera* 2/2020
Five course specialization covering Convolutional Neural Networks, hyperparameter tuning, etc.

Teaching

Rice University, *Houston, TX*

- Taught guest lectures for Algorithmic Robotics (COMP 450), Geometric Methods in Structural Computational Biology (COMP 470), and Biomedical Informatics (COMP 573), several semesters.
- Taught COMP 450, Algorithmic Robotics, Fall 2011.
- Developed a teaching module for motion planning, including a series of assignments and accompanying software (see p. 13).
- Developed and taught an advanced graduate class on control theory for motion planning (see https://moll.ai/control), Spring 2004.
- Coordinated an introductory computational biology seminar, Summer 2003.
- Organized an introductory robotics seminar, Spring 2003.
- Organized a reading group on probabilistic motion planning techniques, Fall 2002.

Carnegie Mellon University, *Pittsburgh, PA*

- Taught guest lectures for Robotic Manipulation, Fall 2001.
- Served as teaching assistant for Robotic Manipulation (Fall 2000) and Computer Graphics (Fall 1998).
- Participated in several workshops organized by the Eberly Center for Teaching Excellence: Overview of Student Motivation, Planning Effective Lectures, Working Well with Small Groups, video observation of a lecture, 1998–2000.

Academic Advising

Thesis Committee Member

Benjamin Tam, PhD, *Adaptive behaviour selection for autonomous robots*, University of Queensland, Australia, March 2023.

Adam Pettinger, PhD, *Using Affordance Primitives to Enhance Robotic Manipulation Task Autonomy and Execution*, University of Texas at Austin, March 2023.

Jeroen De Maeyer, PhD, *Under-constrained end-effector path following: Sampling-based planning algorithms and benchmarking framework*, KU Leuven, November 2021.

Andrew Short, PhD, *Sampling Based Motion Planning with Contacts*, University of Wollongong, June 2020.

Bryce Willey, MS, *Combining Sampling and Optimizing in Robotic Path Planning*, Rice University, August 2018.

Zachary Kingston, MS, *A Unifying Framework for Constrained Sampling-Based Planning*, Rice University, November 2017.

Dave Coleman, PhD, *Methods for Improving Motion Planning Using Experience*, University of Colorado Boulder, December 2016.

Stephen Butler, MS, *General Algorithms for the Time-Optimal Trajectory Generation Problem*, Rice University, November 2016.

Ryan Luna, PhD, *Combining Discrete and Continuous Reasoning for Robot Motion Planning in Complex Domains*, Rice University, May 2016.

Devin Grady, PhD, *Motion Planning with Uncertain Information in Robotic Tasks*, Rice University, December 2013.

Jeffrey Chyan, MS, *Examining the Use of Homology Models in Predicting Kinase Binding Affinity*, Rice University, August 2013.

Ioan Şucan, PhD, *Motion Planning using Task Graphs for Mobile Manipulators*, Rice University, August 2011.

Devin Grady, MS, *Unsynchronized Distributed Motion Planning with Safety Guarantees under Second-Order Dynamics*, Rice University, April 2011.

Research Supervision

Post-docs: Juan David Hernández Vega, Didier Devaurs, Dinler Antunes, Ankur Dhanik, Bryant Gipson, Nurit Haspel.

Graduate students: Bryce Willey, Zachary Kingston, Jayvee Abella, Stephen Butler, Martha Witick, Sarah Kim, Anastasia Novinskaya, Ryan Luna, Jeffrey Chyan, Devin Grady, Ioan Şucan, Drew Bryant, Harris Chiu, David Schwarz, Mili Shah.

Undergraduate students: Thomas Herring, Cary Jiang, Ljubica Vujović, Cannon Lewis, Colin Losey, Sujay Tadwalkar, Prudhvi Boyapalli, Konstantinos Varvarezos, Beck Chen, Caleb Voss, Riya Fukui, Elizabeth Fudge, Christopher Alme, Neal Ehardt, Ricardo Alvarez, Nick Zhu, Nick Bridle, Nicolas Feltman, Allison Heath.

Google Summer of Code students: Jeroen De Maeyer (KU Leuven, 2020), Raghavender Sahdev (York University, Toronto, Canada, 2018), Dave Coleman (U. Colorado, 2014), Javier Gomez (Universidad Carlos III de Madrid, 2014), Luis Torres (UNC Chapel Hill, 2013), Caleb Voss (Rice University, 2013).

Professional Service

- Senior Member of the IEEE, 2013–present.
- Associate Editor for IEEE Robotics and Automation Letters, 2017–2020.
- Moderator for the arXiv Robotics section, 2016–2019.
- Review Manager for the 2014 Robotics Science and Systems (RSS) conference.
- Associate Editor for the Conference Editorial Board of the IEEE International Conference on Robotics and Automation (ICRA) 2015, 2008–2013.
- Associate Editor for the Conference Paper Review Board of the IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS) 2011–2013, 2008.
- Co-organizer of the Workshop on Space Robot Software at the 2023 IEEE Space Mission Challenges for Information Technology / Space Computing Conference (SMC-IT/SCC).
- Co-organizer of the Motion Planning for Mobile Manipulation Tutorial at ICRA 2013.
- Co-organizer of the Robot Motion Planning for Real Robots Tutorial at IROS 2011.
- Co-organizer of the Protein Structure, Kinematics, and Motion Planning Workshop at the 2009 "Robotics: Science & Systems" conference.
- Main organizer of a motion planning tutorial at IROS 2008.
- Main organizer of the Workshop on Self-Reconfigurable Modular Robots at the 2006 "Robotics: Science & Systems" Conference.
- Member of the IEEE Robotics & Automation Society Technical Committees on (1) Algorithms for Planning and Control of Robot Motion, (2) Software Engineering for Robotics and Automation, and (3) Networked Robotics.
- Member of NSF review panels, 2015–2019.

- Program committee member for the following conferences:
  - ROSCON 2021
  - Workshop on the Algorithmic Foundations of Robotics (2018, 2016, 2010, 2008, 2004)
  - Intl. Joint Conf. on Artificial Intelligence (IJCAI) 2016
  - IEEE Intl. Conf. on Bioinformatics and Biomedicine (BIBM) 2015
  - AAAI conference (2013, 2007, 2006),
  - IEEE/RSJ Intl. Conf. on Intelligent Robots and Systems (2006, 2005, 2001)
  - Workshop on Robotics Methods for Struct. and Dynamic Modeling of Molec. Systems (RMMS 2014)
  - Computational Structural Biology Workshop (CSBW 2013–2014).
- Referee for the following journals:
  - AI Communications
  - Algorithmica
  - Annual Review of Control, Robotics, and Autonomous Systems
  - Autonomous Robots
  - BMC Bioinformatics
  - Comp. and Struct. Biotechnology Journal
  - Expert Opinion on Drug Discovery
  - Frontiers in Robotics and AI
  - IEEE/ACM Trans. on Comp. Biology and Bioinf.
  - IEEE Trans. on Robotics
  - IEEE Trans. on Automation Science and Eng.
  - IEEE Trans. on Human-Robot Interaction
  - IEEE Trans. on Systems, Man, and Cybernetics, A
  - IEEE Robotics and Automation Letters
  - IEEE Robotics and Automation Magazine
  - Intl. Journal of Computer Vision
  - Intl. Journal of Robotics Research
  - Intl. Journal of Mechatronics
  - Journal of Computational Biology
  - Journal of Molecular Graphics and Modelling
  - PLOS ONE
  - PLOS Computational Biology
  - Proteins: Structure, Function, and Bioinf.
  - Robotica
  - Robotics and Autonomous Systems
  - Theoretical Computer Science
  - Visual Computer
- Referee for the following conferences:
  - "Robotics: Science and Systems" Conference (2024, 2020, 2018, 2017, 2015, 2013, 2012, 2005–2010)
  - AUVSI XPONENTIAL 2024
  - International Symposium on Robotics Research (ISRR 2017, 2019)
  - IEEE Intl. Conf. on Robotics and Automation (ICRA 2023, 2016–2018, 2010–2014, 2007, 2002–2005)
  - IEEE/RSJ Intl. Conf. on Intelligent Robots and Systems (IROS 2018, 2016, 2012, 2009, 2005–2007, 2001)
  - Humanoids 2015
  - Extreme Science and Engineering Discovery Environment Conf. (XSEDE 2013)
  - 13th International Conference on Ubiquitous Computing (UbiComp 2011)
  - Workshop on Algorithms in Bioinformatics (WABI 2010)
  - American Control Conference (ACC 2010)
  - International Conference on Computational Systems Bioinformatics (CSB 2008, 2007)
  - SIGGRAPH (2007, 2006)
  - Symposium on Computational Geometry (SoCG 2004)
  - International Conference on Research in Computational Molecular Biology (RECOMB 2012, 2003)
  - The Workshop on the Algorithmic Foundations of Robotics (2012)

Publications

Publications are available online at https://moll.ai/publications.

Statistics from Google Scholar: 7,212 citations, *h*-index=32, and i10-index=61.

Refereed Journal Articles

[J38] D. A. Antunes, J. R. Abella, S. Hall-Swan, D. Devaurs, A. Conev, **M. Moll**, G. Lizée, and L. E. Kavraki. HLA-Arena: A customizable environment for the structural modeling and analysis of peptide-HLA complexes for cancer immunotherapy. *JCO Clinical Cancer Informatics*, 4:623–636, 2020. doi:10.1200/CCI.19.00123.

[J37] R. Luna, **M. Moll**, J. M. Badger, and L. E. Kavraki. A scalable motion planner for high-dimensional kinematic systems. *Intl. J. of Robotics Research*, 39(4):361–388, 2020. doi:10.1177/0278364919890408.

[J36] J. D. Hernández, S. Sobti, A. Sciola, **M. Moll**, and L. E. Kavraki. Increasing robot autonomy via motion planning and an augmented reality interface. *IEEE Robotics and Automation Letters*, 5(2):1017–1023, April 2020. doi:10.1109/LRA.2020.2967280.

[J35] S. M. Kim, M. I. Peña, **M. Moll**, G. N. Bennett, and L. E. Kavraki. Improving the organization and interactivity of metabolic pathfinding with precomputed pathways. *BMC Bioinformatics*, 21(1):13, January 2020. doi:10.1186/s12859-019-3328-x.

[J34] Z. Kingston, **M. Moll**, and L. E. Kavraki. Exploring implicit spaces for constrained sampling-based planning. *Intl. J. of Robotics Research*, 38(10–11):1151–1178, September 2019. doi:10.1177/0278364919868530.

[J33] D. Devaurs, D. A. Antunes, S. Hall-Swan, N. Mitchell, **M. Moll**, G. Lizée, and L. E. Kavraki. Using parallelized incremental meta-docking can solve the conformational sampling issue when docking large ligands to proteins. *BMC Molecular and Cell Biology*, 20(1):42, September 2019. doi:10.1186/s12860-019-0218-z.

[J32] E. E. Litsa, M. I. Peña, **M. Moll**, G. Giannakopoulos, G. N. Bennett, and L. E. Kavraki. Machine learning guided atom mapping of metabolic reactions. *Journal of Chemical Information and Modeling*, 59(3):1121–1135, March 2019. doi:10.1021/acs.jcim.8b00434.

[J31] J. D. Hernández, E. Vidal, **M. Moll**, N. Palomeras, M. Carreras, and L. E. Kavraki. Online motion planning for unexplored underwater environments using autonomous underwater vehicles. *Journal of Field Robotics*, 36(2):370–396, March 2019. doi:10.1002/rob.21827.

[J30] Z. Kingston, **M. Moll**, and L. E. Kavraki. Sampling-based methods for motion planning with constraints. *Annual Review of Control, Robotics, and Autonomous Systems*, 1:159–185, May 2018. doi:10.1146/annurev-control-060117-105226.

[J29] Muhayyuddin, **M. Moll**, L. E. Kavraki, and J. Rosell. Randomized physics-based motion planning for grasping in cluttered and uncertain environments. *IEEE Robotics and Automation Letters*, 3(2):712–719, April 2018. doi:10.1109/LRA.2017.2783445.

[J28] D. A. Antunes, D. Devaurs, **M. Moll**, G. Lizée, and L. E. Kavraki. General prediction of peptide-MHC binding modes using incremental docking: A proof of concept. *Scientific Reports*, 8(1):4327, March 2018. doi:10.1038/s41598-018-22173-4.

[J27] D. Devaurs, M. Papanastasiou, D. Antunes, J. Abella, **M. Moll**, D. Ricklin, J. Lambris, and L. E. Kavraki. Native state of complement protein C3d analyzed via hydrogen exchange and conformational sampling. *Intl. J. of Computational Biology and Drug Design*, 11(1/2):90–113, March 2018. doi:10.1504/IJCBDD.2018.10011903. Special issue on the 2016 Intl. Conf. on Intelligent Biology and Medicine (ICIBM).

[J26] J. R. Abella, **M. Moll**, and L. E. Kavraki. Maintaining and enhancing diversity of sampled protein conformations in robotics-inspired methods. *Journal of Computational Biology*, 25(1):3–20, January 2018. doi:10.1089/cmb.2017.0164.

[J25] D. A. Antunes, **M. Moll**, D. Devaurs, K. Jackson, G. Lizée, and L. E. Kavraki. DINC 2.0: a new protein-peptide docking webserver using an incremental approach. *Cancer Research*, 77(21):e55–57, November 2017. doi:10.1158/0008-5472.CAN-17-0511.

[J24] S. M. Kim, M. I. Peña, **M. Moll**, G. N. Bennett, and L. E. Kavraki. A review of parameters and heuristics for guiding metabolic pathfinding. *Journal of Cheminformatics*, 9(1):51, September 2017. doi:10.1186/s13321-017-0239-6.

[J23] D. Devaurs, D. A. Antunes, M. Papanastasiou, **M. Moll**, D. Ricklin, J. D. Lambris, and L. E. Kavraki. Coarse-grained conformational sampling of protein structure improves the fit to experimental hydrogen-exchange data. *Frontiers in Molecular Biosciences*, 4(13), March 2017. doi:10.3389/fmolb.2017.00013.

[J22] A. Novinskaya, D. Devaurs, **M. Moll**, and L. E. Kavraki. Defining low-dimensional projections to guide protein conformational sampling. *Journal of Computational Biology*, 24(1):79–89, January 2017. doi:10.1089/cmb.2016.0144. (A preliminary version of this article was first published as a conference paper; see below.).

[J21] **M. Moll**, P. W. Finn, and L. E. Kavraki. Structure-guided selection of specificity determining positions in the human kinome. *BMC Genomics*, 17 (Suppl. 4):431, August 2016. doi:10.1186/s12864-016-2790-3. (A preliminary version of this article was first published as a conference paper; see below.).

[J20] L. E. Kavraki and **M. Moll**. Special issue on the 2014 "Robotics: Science & Systems" conference (guest editorial). *Intl. J. of Robotics Research*, 35(1–3):3–4, March 2016. doi:10.1177/0278364915608299.

[J19] **M. Moll**, I. A. Şucan, and L. E. Kavraki. Benchmarking motion planning algorithms: An extensible infrastructure for analysis and visualization. *IEEE Robotics & Automation Magazine (Special Issue on Replicable and Measurable Robotics Research)*, 22(3):96–102, September 2015. doi:10.1109/MRA.2015.2448276.

[J18] D. K. Grady, **M. Moll**, and L. E. Kavraki. Extending the applicability of POMDP solutions to robotic tasks. *IEEE Trans. on Robotics*, 31(4):948–961, August 2015. doi:10.1109/TRO.2015.2441511.

[J17] **M. Moll**, J. Bordeaux, and L. E. Kavraki. Software for project-based learning of robot motion planning. *Computer Science Education, Special Issue on Robotics in CS Education*, 23(4):332–348, 2013. doi:10.1080/08993408.2013.847167.

[J16] B. Gipson, **M. Moll**, and L. E. Kavraki. SIMS: A hybrid method for rapid conformational analysis. *PLOS ONE*, 8(7):e68826, July 2013. doi:10.1371/journal.pone.0068826.

[J15] D. H. Bryant, **M. Moll**, P. W. Finn, and L. E. Kavraki. Combinatorial clustering of residue position subsets predicts inhibitor affinity across the human kinome. *PLOS Computational Biology*, 9(6):e1003087, June 2013. doi:10.1371/journal.pcbi.1003087.

[J14] I. A. Şucan, **M. Moll**, and L. E. Kavraki. The Open Motion Planning Library. *IEEE Robotics & Automation Magazine*, 19(4):72–82, December 2012. doi:10.1109/MRA.2012.2205651. http://ompl.kavrakilab.org.

[J13] K. E. Bekris, D. K. Grady, **M. Moll**, and L. E. Kavraki. Safe distributed motion coordination for second-order systems with different planning cycles. *Intl. J. of Robotics Research*, 31(2):129–149, February 2012. doi:10.1177/0278364911430420.

[J12] **M. Moll**, D. H. Bryant, and L. E. Kavraki. The LabelHash server and tools for substructure-based functional annotation. *Bioinformatics*, 27(15):2161–2162, June 2011. doi:10.1093/bioinformatics/btr343.

[J11] **M. Moll**, J. Bordeaux, and L. E. Kavraki. Teaching robot motion planning. *ASEE Computers in Education Journal (Special Issue on Novel Approaches to Robotics Education)*, 20(3):50–59, 2010. URL: https://www.asee.org/papers-and-publications/publications/division-publications/computers-in-education-journal/volume-xx.

[J10] N. Haspel, **M. Moll**, M. L. Baker, W. Chiu, and L. E. Kavraki. Tracing conformational changes in proteins. *BMC Structural Biology*, 10(Suppl. 1):S1, 2010. doi:10.1186/1472-6807-10-S1-S1. (A preliminary version of this article was first published as a conference paper; see below.).

[J9] **M. Moll**, D. H. Bryant, and L. E. Kavraki. The LabelHash algorithm for substructure matching. *BMC Bioinformatics*, 11(555), November 2010. doi:10.1186/1471-2105-11-555.

[J8] D. H. Bryant, **M. Moll**, B. Y. Chen, V. Y. Fofanov, and L. E. Kavraki. Analysis of substructural variation in families of enzymatic proteins with applications to protein function prediction. *BMC Bioinformatics*, 11 (242), May 2010. doi:10.1186/1471-2105-11-242. **Evaluated on the Faculty of 1000 web site.**

[J7] **M. Moll** and D. Rus. Special issue on self-reconfiguring modular robots (guest editorial). *Intl. J. of Robotics Research*, 27(3/4):277–278, March/April 2008. doi:10.1177/0278364908089348.

[J6] M. Yim, W.-M. Shen, B. Salemi, D. Rus, **M. Moll**, H. Lipson, and E. Klavins. Modular self-reconfigurable robot systems: Challenges and opportunities for the future. *IEEE Robotics & Automation Magazine*, 14(1): 43–52, March 2007. doi:10.1109/MRA.2007.339623.

[J5] **M. Moll** and L. E. Kavraki. Path planning for deformable linear objects. *IEEE Trans. on Robotics*, 22(4): 625–636, August 2006. doi:10.1109/TRO.2006.878933.

[J4] P. Das, **M. Moll**, H. Stamati, L. E. Kavraki, and C. Clementi. Low-dimensional, free-energy landscapes of protein-folding reactions by nonlinear dimensionality reduction. *Proc. Natl. Acad. of Science USA*, 103(26): 9885–9890, June 2006. doi:10.1073/pnas.0603553103.

[J3] **M. Moll** and M. A. Erdmann. Manipulation of pose distributions. *Intl. J. of Robotics Research*, 21(3):277–292, March 2002. doi:10.1177/027836402320556449.

[J2] **M. Moll**, K. Goldberg, M. A. Erdmann, and R. Fearing. Aligning parts for micro assemblies. *Assembly Automation*, 22(1):46–54, February 2002. doi:10.1108/01445150210416673.

[J1] **M. Moll** and R. Miikkulainen. Convergence-zone episodic memory: Analysis and simulations. *Neural Networks*, 10(6):1017–1036, August 1997. doi:10.1016/S0893-6080(97)00016-6.

Book Chapters

[B6] Z. Kingston, **M. Moll**, and L. E. Kavraki. Decoupling constraints from sampling-based planners. In N. M. Amato, G. Hager, S. Thomas, and M. Torres-Torriti, editors, *Robotics Research (The 18th International Symposium ISRR)*, pages 913–928. Springer, 2020. doi:10.1007/978-3-030-28619-4_62.

[B5] S. Butler, **M. Moll**, and L. E. Kavraki. A general algorithm for time-optimal trajectory generation subject to minimum and maximum constraints. In K. Goldberg, P. Abbeel, K. Bekris, and L. Miller, editors, *Algorithmic Foundations of Robotics XII*, pages 368–383. Springer, 2020. doi:10.1007/978-3-030-43089-4_24.

[B4] R. Luna, M. Lahijanian, **M. Moll**, and L. E. Kavraki. Asymptotically optimal stochastic motion planning with temporal goals. In H. L. Akin, N. M. Amato, V. Isler, and A. F. van der Stappen, editors, *Algorithmic Foundations of Robotics XI*, volume 107 of *Springer Tracts in Advanced Robotics*, pages 335–352. Springer Verlag, 2015. doi:10.1007/978-3-319-16595-0_20.

[B3] **M. Moll**, D. Schwarz, and L. E. Kavraki. Roadmap methods for protein folding. In M. Zaki and C. Bystroff, editors, *Protein Structure Prediction: Methods and Protocols*, Methods In Molecular Biology. Humana Press, second edition, October 2007. doi:10.1007/978-1-59745-574-9_9.

[B2] **M. Moll** and M. A. Erdmann. Reconstructing the shape and motion of unknown objects with active tactile sensors. In J.-D. Boissonnat, J. Burdick, K. Goldberg, and S. Hutchinson, editors, *Algorithmic Foundations of Robotics V*, Springer Tracts in Advanced Robotics, pages 293–310. Springer Verlag, 2004. doi:10.1007/b80173.

[B1] **M. Moll** and M. A. Erdmann. Manipulation of pose distributions. In B. R. Donald, K. M. Lynch, and D. Rus, editors, *Algorithmic and Computational Robotics: New Directions*, pages 127–141. A. K. Peters, 2001. URL: http://www.crcpress.com/product/isbn/9781568811253.

Refereed Conference Papers

[C44] **M. Moll**. 3D Dubins paths for underwater vehicles. In *Proc. IEEE/MTS Oceans Conf.*, Halifax, Canada, 2024. doi:10.1109/OCEANS55160.2024.10754581.

[C43] **M. Moll**. A general framework for remote command and control of robots in space. In *AIAA Scitech 2023 Forum*, National Harbor, MD, January 2023. doi:10.2514/6.2023-1069.

[C42] **M. Moll**, C. Chamzas, Z. Kingston, and L. E. Kavraki. HyperPlan: A framework for motion planning algorithm selection and parameter optimization. In *IEEE/RSJ Intl. Conf. on Intelligent Robots and Systems*, pages 2511–2518, 2021. doi:10.1109/IROS51168.2021.9636651.

[C41] Z. Kingston, A. M. Wells, **M. Moll**, J. M. Badger, and L. E. Kavraki. Informing multi-modal planning with synergistic discrete leads. In *IEEE Intl. Conf. on Robotics and Automation*, 2020. doi:10.1109/ICRA40945.2020.9197545.

[C40] E. Vidal Garcia, **M. Moll**, N. Palomeras, J. D. Hernández, M. Carreras, and L. Kavraki. Online multilayered motion planning with dynamic constraints for autonomous underwater vehicles. In *IEEE Intl. Conf. on Robotics and Automation*, pages 8936–8942, May 2019. doi:10.1109/ICRA.2019.8794009. **Finalist for best student paper award**.

[C39] J. D. Hernández, **M. Moll**, and L. E. Kavraki. Lazy evaluation of goal specifications guided by motion planning. In *IEEE Intl. Conf. on Robotics and Automation*, pages 944–950, May 2019. doi:10.1109/ICRA.2019.8793570.

[C38] W. Baker, Z. Kingston, **M. Moll**, J. Badger, and L. Kavraki. Robonaut 2 and you: Specifying and executing complex operations. In *IEEE Workshop on Advanced Robotics and its Social Impacts (ARSO)*, Austin, TX, March 2017. doi:10.1109/ARSO.2017.8025204.

[C37] J. D. Hernández, **M. Moll**, E. Vidal Garcia, M. Carreras, and L. E. Kavraki. Planning feasible and safe paths online for autonomous underwater vehicles in unknown environments. In *IEEE/RSJ Intl. Conf. on Intelligent Robots and Systems*, pages 1313–1320, October 2016. doi:10.1109/IROS.2016.7759217.

[C36] S. M. Kim, M. I. Peña, **M. Moll**, G. Giannakopoulos, G. N. Bennett, and L. E. Kavraki. An evaluation of different clustering methods and distance measures used for grouping metabolic pathways. In *Eighth International Conference on Bioinformatics and Computational Biology (BICoB)*, April 2016.

[C35] A. Novinskaya, D. Devaurs, **M. Moll**, and L. E. Kavraki. Improving protein conformational sampling by using guiding projections. In *IEEE Intl. Conf. on Bioinformatics and Biomedicine Workshops (BIBMW)*, pages 1272–1279, November 2015. doi:10.1109/BIBM.2015.7359863.

[C34] **M. Moll**, P. W. Finn, and L. E. Kavraki. Structure-guided selection of specificity determining positions in the human kinome. In *IEEE International Conference on Bioinformatics and Biomedicine (BIBM)*, pages 21–28, November 2015. doi:10.1109/BIBM.2015.7359650. **Winner of the best paper award.**

[C33] C. Voss, **M. Moll**, and L. E. Kavraki. A heuristic approach to finding diverse short paths. In *IEEE Intl. Conf. on Robotics and Automation*, pages 4173–4179, May 2015. doi:10.1109/ICRA.2015.7139774.

[C32] D. Coleman, I. A. Şucan, **M. Moll**, K. Okada, and N. Correll. Experience-based planning with sparse roadmap spanners. In *IEEE Intl. Conf. on Robotics and Automation*, pages 900–905, May 2015. doi:10.1109/ICRA.2015.7139284.

[C31] R. Luna, M. Lahijanian, **M. Moll**, and L. E. Kavraki. Fast stochastic motion planning with optimality guarantees using local policy reconfiguration. In *IEEE Intl. Conf. on Robotics and Automation*, pages 3013–3019, 2014. doi:10.1109/ICRA.2014.6907293.

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Invited Talks

- The University of North Carolina at Charlotte, November 15, 2024. *Multilayered Planning for Autonomous Underwater Vehicles.*
- Lunar Surface Innovation Consortium Mobility Technology Subgroup, May 25, 2023. *A General Framework for Remote Command and Control of Robots in Space.*
- Lunar Surface Innovation Consortium Extreme Access Focus Group, May 11, 2023. *A General Framework for Remote Command and Control of Robots in Space.*
- NASA JPL seminar, Pasadena, CA. December 7, 2022. *A General Framework for Remote Command and Control of Robots in Space.*
- IROS 2022 Workshop on Evaluating Motion Planning Performance, Kyoto, Japan. October 23, 2022. *Using Hyperparameter Optimization for Motion Planning Algorithm Configuration.*
- Georgia Tech Institute for Robotics and Intelligent Machines Seminar, Atlanta, GA. January 26, 2022. *Robot Motion Planning: Challenges and Opportunities for Increasing Robot Autonomy.*
- Galois, Portland, OR. May 28, 2021. *Toward Robot Autonomy: Tasks, Plans, and Policies.*
- Texas System Day, Texas A&M, College Station, TX. April 5, 2019. *Toward Robot Autonomy: Tasks, Plans, and Policies.*
- Workshop on Automation, AI & Robotics, NASA Johnson Space Center, Houston, TX. March 27, 2019. *Robot Motion Planning: Challenges and Opportunities for Increasing Robot Autonomy.*
- First Summer School on Cognitive Robotics, Massachusetts Institute of Technology, Cambridge, MA. June 13, 2017. *Sampling-Based Motion Planning.*
- University of Houston at Clear Lake. September 7, 2016. *Motion Planning: From Robots to Molecules.*
- Intl. Conf. on Automated Planning and Scheduling (ICAPS) Summer School, King's College, London, UK. June 9, 2016. *Sampling-based motion planning and its combination with task planning.*
- University of Twente, the Netherlands. March 27, 2015. *Computing Robot Motion Plans from High-Level Specifications.*
- University of Utrecht, the Netherlands. March 26, 2015. *Computing Robot Motion Plans from High-Level Specifications.*
- University of Utrecht, the Netherlands. March 26, 2015. *Modeling Conformational Changes in Large Molecular Complexes.*
- Networking event for alumni of Dutch polytechnical universities, Houston, TX. November 21, 2014. *Motion Planning: From Robots to Molecules*
- Workshop on Robotics Methods for Structural and Dynamic Modeling of Molecular Systems at the Robotics Science & Systems (RSS) conference, July 12, 2014. *Motion Planning for Large Molecular Complexes.*
- Open Source Software World Challenge Awards Day, Seoul, Korea. November 27, 2012. *The Open Motion Planning Library.*
- HPC Workshop, Rice University. October 1, 2008. *HPC for Computational Structural Biology.*
- Texas A&M University. November 16, 2007. *Nonlinear Dimensionality Reduction for the Analysis of Protein Motion.*
- Information Sciences Institute, University of Southern California. May 21, 2005. *Manipulation and Shape Modeling for Robotics Applications.*
- Intl. Workshop on Motion Planning in Virtual Environments, Toulouse, France. January 8, 2005. *Applying Motion Planning Techniques to Molecular Docking.*

- Honda Research Institute, USA. December 13, 2004. *Manipulation and Shape Modeling for Robotics Applications.*
- NASA Johnson Space Center. April 7, 2004. *Shape Reconstruction Using Active Tactile Sensors.*
- NASA Ames Research Center. March 10, 2004. *Shape Reconstruction Using Active Tactile Sensors.*
- INRIA Sophia-Antipolis, France. December 20, 2002. *Nonprehensile Manipulation and Sensing.*
- Univ. of Mass. at Amherst. March 2, 2002. *Shape Reconstruction Using Active Tactile Sensors.*
- Texas A&M University. March 21, 2002. *Shape Reconstruction Using Active Tactile Sensors.*
- Johns Hopkins University. March 28, 2002. *Shape Reconstruction Using Active Tactile Sensors.*
- Center for the Neural Basis of Cognition Brain Bag Seminar, Carnegie Mellon University. November 25, 1996. *Convergence-Zone Episodic Memory: Analysis and Simulations.*
- Parallel Distributed Processing Group Meeting, Psychology Department, Carnegie Mellon University. November 15, 1996. *Convergence-Zone Episodic Memory: Analysis and Simulations.*

Selected Funding

- **NASA SBIR Phase III 80NSSC23CA026,** 2023–2024, $375,000, Principal Investigator. *Improved Capabilities for Dexterous Robot Platforms with MoveIt Studio.*
- **NASA SBIR Phase I/II 80NSSC22PB156,** 2022–2024, $1,006,487, Principal Investigator. *An Affordance Driven, Human-in-the-Loop Perception Framework.*
- **SpaceWERX Orbital Prime FA8750-22-C-0093,** 2022-2023, $249,990, Principal Investigator. *Integrated Planning and Control for On-Orbit Capture.*
- **Colorado Advanced Industries,** 2022–2023, $250,000, Principal Investigator.
- **NASA SBIR Phase I/II/II-E 80NSSC21C0539,** 2021–2024, $1,129,997, Principal Investigator. *Advanced planning capabilities for robots in microgravity environments.*
- **NASA NNX15AI58G,** 2015–2016, $40,000, Co-Principal Investigator. *Planning high-quality motions for Robonaut 2*
- **NSF IIS 1317849,** 2013–2019, $923,140, Co-Principal Investigator. *Rethinking Motion Generation for Robots Operating in Human Workspaces.*
- **NASA NNX13AD09G,** 2012–2013, $30,000, Co-Principal Investigator. *Locomotion strategies for the legs of Robonaut 2*

I have also co-authored the proposals below and worked as senior personnel on them:

- **NASA SBIR Phase 1,** 2023–2024, $150,000. *A Framework for Failure Management and Recovery for Remote Autonomous Task Planning and Execution.*
- **NSF IIS 1830549,** 2018–2021, $749,291. *Robotic Collaboration through Scalable Reactive Synthesis.*
- **CPRIT RP170508,** 2016–2019, $900,000. *Structural modeling of peptide-HLA complexes presenting a melanoma-associated antigen for cross-reactivity assessment.*
- **NSF CCF 1514372,** 2015–2019, $815,999. *Automating robot programming through constraint solving and motion planning.*
- **NSF CCF 1423304,** 2014–2017, $458,128. *An Integrated Approach to Characterizing Conformational Changes of Large Proteins.*
- **NSF DBI 1262491,** 2013–2019, $694,873. *Mining Metabolic and Enzyme Databases for the Composition of Non-Canonical Pathways.*
- **NSF DBI 0960612,** 2010–2016, $765,686. *A Toolbox for Large-Scale Analysis of Structural Molecular Data.*

- **NSF DUE 0920721,** 2009–2014, $250,000. *Teaching robot motion planning through an integrated software environment.*
- **DOD Army RDECOM W911NF-09-1-0383,** 2009–2015, $7,500,000. *Opportunistic Sensing.*
- **NIH R01 GM078988,** 2006–2010, $717,796. *Dimensionality Reduction and Search for Analyzing Protein Structure.*

Scientific Software

- **The Open Motion Planning Library** (https://ompl.kavrakilab.org): a library containing implementations of many motion planning algorithms, as well as a simple GUI. With Ioan Şucan and many other developers. Used inside the Robot Operating System (ROS) and several other robotics software packages. **Winner of the 2012 Open Source Software World Challenge.**
- **MoveIt** (https://moveit.ros.org): widely used software for robotic manipulation and motion planning. It has been used on over 126 robots. I am one of its maintainers.
- **The DINC Server** (http://dinc.kavrakilab.org): a web server for incremental molecular docking of large ligands and peptides. This is joint work with Dinler Antunes, Didier Devaurs, Ankur Dhanik and several others.
- **LabelHash** (http://labelhash.kavrakilab.org): a system that, given a small 3D protein substructure, finds all substructures in a large collection of proteins that are geometrically and chemically similar to it. With Drew Bryant.
- **MacPorts** (https://www.macports.org): maintainer of a number of scientific software ports for MacPorts, an Open Source package manager for macOS.