Curriculum Vitæ

Bruce Randall Donald
James B. Duke Distinguished Professor
of Computer Science and Mathematics, Chemistry and Biochemistry
Duke University

December 26, 2024

Contents

1 Principal Fields of Interest

Computational Molecular Biology.

>>Algorithms in Structural Molecular Biology.
>>Computational Chemistry.
>>Protein and Molecular Design.
>>Systems Biology.

Structural Biology & Biochemistry.
Microelectromechanical Systems (MEMS) and Nanoscience.
Artificial Intellgence

>>Machine Learning
>>Robotics

Geometric & physical algorithms.

2 Education

Ph.D in Computer Science, Massachusetts Institute of Technology, 1987. Department of Electrical Engineering and Computer Science.
>Research laboratory: MIT Artificial Intelligence Laboratory.[1]
>Minor: Mathematics (Topology).
>Oral exam committee: Patrick Winston, Michael Sipser, Sanjoy Mitter.
>Dissertation committee: Tomás Lozano-Pérez (Advisor), Rod Brooks, Eric Grimson.

S.M. in Electrical Engineering and Computer Science, Massachusetts Institute of Technology, 1984. Area: Computer Science.
>Research laboratory: MIT Artificial Intelligence Laboratory.
>Advisor: Professor Tomás Lozano-Pérez.

B.A. *Summa cum laude,* with Distinction in the Major, Yale University, 1980.[2]

Special Student, Graduate School of Arts & Sciences, Harvard University, 1975-76.[3]

3 Professional Experience

Note: This section lists academic experience (past and present), and current industry positions. For previous industry experience and consulting, see §5.

(2012—   ) James B. Duke Distinguished Professor of Computer Science, Duke University.
(2020—   ) Professor of Mathematics, Duke University.
(2020—   ) Founder and Chairman, Scientific Advisory Board, Ten63 Therapeutics, Inc.
(2014—   ) Professor of Chemistry, Duke University.
(2006—   ) Professor of Biochemistry, School of Medicine, Duke University Medical Center.
(2010—2021) Professor of Electrical and Computer Engineering, Pratt School of Engineering, Duke University.
(2006—2012) William and Sue Gross Professor of Computer Science, Duke University.
(2003—2006) Joan P. and Edward J. Foley Jr 1933 Professor, Dartmouth College.
(1999—2006) Professor of Computer Science, Dartmouth College.
(2000—2006) Adjunct Professor of Chemistry, Dartmouth College.
(2002—2006) Adjunct Professor of Biological Sciences, Dartmouth College.
(1997—1999) Associate Professor (with tenure), Computer Science Department, Dartmouth College.

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[1]The MIT AI Lab (1959–2003) merged with the MIT Lab for Computer Science (LCS) to form CSAIL (Computer Science and Artificial Intelligence Lab) in 2003.

[2]Other Yale honors, awards, etc. are listed in §4 below.

[3]Non-degree program.

(1993—1998) Associate Professor (with tenure), Computer Science Department, Cornell University.
(1987—1993) Assistant Professor, Computer Science Department, Cornell University.

(1984) Research Staff, Artificial Intelligence Laboratory, Massachusetts Institute of Technology.
(1978–84) Laboratory for Computer Graphics and Spatial Analysis, Graduate School of Design, Harvard University, Cambridge, MA. Most senior title: Research Analyst in Computer Graphics and Spatial Analysis (1982-1984).

4 Awards and Honors

NIH Oustanding Investigator Grant. NIH NIGMS R35 EI MIRA Award (2022–   ).
IEEE Life Fellow (2024).
PLOS ONE Editorial Board Long Service Award (2023).
Fellow of the AAAS (American Association for the Advancement of Science) (2015–   ).
Fellow of the IEEE (2011–   ).
Fellow of the Association for Computing Machinery (ACM) (2009–   ).
John Simon Guggenheim Memorial Fellow (2001–2002).
National Science Foundation Presidential Young Investigator (1989–1994).
NASA/Jet Propulsion Laboratory (JPL) Graduate Student Researcher Fellowship (1985-1987).
Phi Beta Kappa, Yale University (1979).
Wallace Fiction Prize, Yale University (1978). (Peter J. Wallace Memorial Prize for short story writing).
J. Edward Meeker Prize for Writing, Yale University (1977).
See also §2, above for Latin honors, etc.

4.1 Honorary Degree

A.M. (Hon.) Dartmouth College, 2000.
Dartmouth confers an A.M. degree *"Ut in grege nostro numeretur"* on faculty members appointed to full professor.[4]

4.2 University Awards

AI for Art Competition, Duke University, Second prize (2022).
Bass Society of Fellows, Duke University (2006–   ).
Edward and Joan Foley Fellow, Dartmouth College (2000–2001).
Senior Faculty Grant, Dartmouth College (2001).
Friedman Faculty Fellow, Dartmouth College (1999–2000).

4.3 Distinguished and Inaugural Lectures

Computer Science Department Distinguished Lecture. Tulane University (2013).
Inaugural Lecture, Nanotechnology Public Lecture Series, MIT (2007).
Robert Mueller-Thuns Distinguished Lecture in Computer Science, the University of Illinois at Urbana-Champaign (2002).
Triangle Distinguished Lecture in Computer Science, University of North Carolina at Chapel Hill, Duke, and N. C. State (2002).

4.4 Selected Best Paper/Poster Awards

Top Downloaded Paper, 2018-19 *Journal of Computational Chemistry*: "OSPREY 3.0: Open-Source Protein Redesign for You, with Powerful New Features." See Publication #12 in §14.2.2 below.

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[4]This tradition may have been modeled on Harvard's. *cf.* Elkins, Kimball C. "Honorary Degrees at Harvard." Harvard Library Bulletin Volume XII Number 3 (Autumn 1958): 326-353. `http://pds.lib.harvard.edu/pds/view/2573358?n=5505&s=4`

Best Poster Award at the Structural Bioinformatics and Computational Biophysics (3DSIG), ISMB Satellite Meeting, Boston, MA July 11-12, 2014.

Best Paper Award at the *Computational Systems Bioinformatics Conference (CSB 2006)*.

The Faculty of 1000 selected our paper in *Journal of Biological Chemistry*, 2003 (see §14.2.2). The paper was rated "exceptional," with a rating of 9.0, and appeared as #1 in the Hidden Jewels Top 10 of Microbiology category.

Best Poster Award at the *Computational Systems Bioinformatics Conference (CSB 2003)* sponsored by the IEEE Computer Society in cooperation with the ACM.

Finalist for Best Paper Award, *IEEE International Conference on Robotics and Automation,* (1994).

5 Previous Industry Experience and Consulting

Ten63 Therapeutics, Inc. (2020):

> Founder.
> Chief Scientific Officer.
> Corporate Secretary.

Gavilán Biodesign, Inc. (2018—2020):

> Founder.
> Chief Scientific Officer.
> Board of Directors.
> Corporate Secretary.

Member, Scientific Advisory Board, Carta Proteomics, Inc. (now called ExSAR). (2000–2002).

Consultant, Carta Proteomics Inc. (2000–2001).

Founding Fellow, Geniisis Agents (Geniisis LLC, San Francisco) (1999–2003).

Contractor and Consultant, Interval Research Corporation (1995–1997). Co-inventor of Embedded Constraint Graphics (See §14.4, "Patents" and SIGGRAPH'2000 paper in §14.6).

Consultant, Xerox Palo Alto Research Center (1990).

Consultant, Consortium for Mathematics and Its Applications, Lexington, MA. (1980's)

6 Sabbaticals and Leaves

(2009–2010) Visiting Professor, Computer Science Department, University of North Carolina, Chapel Hill.

(2000–2001) Visiting Scientist, Massachusetts Institute of Technology Artificial Intelligence Laboratory and Department of Electrical Engineering and Computer Science.

(1994—1996) Visiting Professor, Computer Science Department, Stanford University.

(1995—1996) Interval Research Corporation, Palo Alto, CA.

7 Student Employment

(1984) Teaching Assistant (recitation instructor) for 6.034, *Artificial Intelligence*, Massachusetts Institute of Technology; in charge: Profs. P. H. Winston, R. C. Berwick, T. Lozano-Pérez.

(1982—1987) Research assistant, Artificial Intelligence Laboratory, Massachusetts Institute of Technology.

8 Professional Activities

Reviewer/Referee for *PNAS, PLoS Computational Biology, Nature Structural & Molecular Biology, Nature Chemical Biology, Nature Methods, Cell Chemical Biology, Proteins, Chemistry & Biology, Journal of Chemical Theory & Computation (JCTC), Protein Science, Journal of Chemical Information and Modeling, Jour. Am. Chem. Soc. (JACS), Human Frontiers of Science Program, Jour. Structural Biology, PLoS One, Journal of Biomolecular NMR,* Programming Language Design and Implementation

(PLDI), *Molecular BioSystems*, European Conference on Computational Biology (ECCB), *Biochimica et Biophysica Acta (BBA) – Proteins and Proteomics*, *Proceedings of the IEEE*, J. Computational Biology, RECOMB, *Bioinformatics*, *Cancer Research*, *J. Physical Chemistry*, *J. Medicinal Chemistry*, *Molecular Cancer Therapeutics*, *Protein Engineering, Design, and Selection*, International Journal of Peptide Research and Therapeutics (Springer), Journal of Bioinformatics and Computational Biology, IEEE/ACM Transactions on Computational Biology and Bioinformatics, IEEE (PAMI, SMC, ICRA, TRA), J. Molecular Graphics and Modelling, AAAI, IJCAI, Int. Jour. Robotics Research, NSF, NIH, Wellcome Trust (UK), Marsden Fund (NZ), Springer-Verlag, Harvard University Press, *Discrete and Computational Geometry*, *Algorithmica*, ACM STOC, ACM SCOG, SIGGRAPH, Int. Jour. of Computational Geometry and Applications, *J. Computer and System Sciences*, Swiss National Science Foundation, German-Israeli Foundation for Scientific Research and Development, *Fonds zur Förderung der wissenschaftlichen Forschung*, FWF (Austrian Science Fund), Volkswagenstiftung Förderung.

Subject Matter Expert (SME), SAGE Program (Science Advice and Guidance for Emergencies), SPCO (Security, Preparedness, Continuity Office), Directorate of Science and Technology (S&T), DHS (Department of Homeland Security) (2024–   ).

Member, Transformative Research Award Special Emphasis Panel/Review Group 2024/05 ZRG1 BTC-Q (70) R, National Institutes of Health. February, 2024.

Editor, *Frontiers in Molecular Biosciences.* Special issue on Biological Modeling and Simulation, with Research Topic: Advances in Computational and Data-Driven Protein Design—Methods and Applications (2021–2023). Published in Volume 9 (2023).

Member, ESI R35 MIRA Study Section, Special Emphasis Panel/Scientific Review Group 2023/05 ZRG1 MBBC-S (54), National Institutes of Health. March, 2023.

Program committee, 21st European Conference on Computational Biology (ECCB), Barcelona 2022.

Member, Novel therapeutics directed to intracellular HIV targets, Special Emphasis Panel ZAI1 RB-A (S5), National Institutes of Health. July, 2020.

Reviewer, NIH Director's New Innovator Award Review (DP2), Special Emphasis Panel ZRG1 MOSS-R (70) R, National Institutes of Health. December 2019/March 2020.

Invited speaker, 35th International Symposium on Computational Geometry (SoCG 2019), Portland, OR. June 21, 2019.

Temporary Member, Macromolecular Structure and Function D Study Section (MSFD), Biological Chemistry and Macromolecular Biophysics (BCMB) Integrated Review Group (IRG), National Institutes of Health. Feb. 7, 2018.

Reviewer, Transformative Research Award Special Emphasis Panel ZRG1-BCMB-A(51)R, Biological Chemistry and Macromolecular Biophysics (BCMB) Integrated Review Group (IRG), National Institutes of Health. February, 2018.

My lab mentored:

The iGEM (International Genetically-Engineered Machines) Team, East Chapel Hill High School (2018), Chapel Hill, NC. Project: "Chloramphenicol acetyltransferase operon for an improved Fluoride Riboswitch as a Technology to Combat Excess Fluoride in Water."

The iGEM Team, East Chapel Hill High School (2017), Chapel Hill, NC. Project: "Developing a Fluoride Riboswitch as a Technology to Combat Excess Fluoride in Water" (with Brian Kuhlman, UNC).

Keynote speaker, Structural Bioinformatics and Computational Biophysics (3DSIG), ISMB Satellite Meeting, Orlando, Fl. July 8, 2016.

Invited speaker, 2nd Protein Engineering Canada (PEC) Conference, Ottawa, ON. June 18, 2016.

Invited speaker, Experimental NMR Conference (ENC). Pittsburgh, PA. April 12, 2016.

Guest editor, *PLoS Computational Biology* (2019).

Editorial Board (Academic Editor), *PLoS One* (2012–   ).

Member, Advisory Committee for Cyberinfrastructure (ACCI), National Science Foundation (NSF) (2012–2014).

Reviewer, Molecular Biophysics Program, National Science Foundation (NSF) (2016).

Reviewer, Chemistry Division, National Science Foundation (NSF) (Spring, 2014; Fall 2014).

Reviewer, Transformative Research Award Special Emphasis Panel 2014/05 ZRG1 BCMB-A (51), Biological Chemistry and Macromolecular Biophysics (BCMB) Integrated Review Group (IRG), National Institutes of Health, February 2014.

Temporary Member, Macromolecular Structure and Function D Study Section (MSFD), Biological Chemistry and Macromolecular Biophysics (BCMB) Integrated Review Group (IRG), National Institutes of Health, December 2 and December 9, 2013.

Program committee, International Conference on Research in Computational Molecular Biology (RE-COMB). Los Angeles, CA (April, 2016).

Program committee, International Conference on Intelligent Systems for Molecular Biology (ISMB):

> Orlando, Florida, July 8-12, 2016.
> Dublin, Ireland. July, 2015.
> Boston, MA. July 11-15, 2014.
> Berlin, Germany. July, 2013.
> Long Beach, CA. July 15-17, 2012.
> Vienna, Austria 2011.
> Boston, MA 2010.

Nominator/Reviewer, MacArthur Fellows Program, The John D. and Catherine T. MacArthur Foundation (2003, 2005, 2016).

Moderator, Computing Research Repository — `arXiv.org` e-Print archive, (Robotics) (1998 – 2016).

Invited Lecture (with C. Levey and I. Paprotny). "Microrobot Species: a Surface MEMS Perspective." IEEE International Conference on Robotics and Automation (ICRA) Workshop on Microrobotics, Karlsruhe, Germany. May 6-10, 2013.

Scientific Program Committee, Scientific Committee of the Workshop on Distance Geometry and Applications (DGA 2013), Brazil. June, 2013.

Keynote speaker, Tenth International Workshop on the Algorithmic Foundations of Robotics (WAFR), CSAIL, MIT, Cambridge, MA. June 13, 2012.

Editorial Board (Associate Editor), *IEEE/ACM Transactions on Computational Biology and Bioinformatics (TCBB)* (2012–2013).

Program committee, *Festschrift* Symposium for Dexter Kozen, Cornell University (2011-2012). Published by Springer-Verlag Lecture Notes in Computer Science (2012).

Program committee, ASE/IEEE International Conference on BioMedical Computing (BioMedCom), Washington D.C., December 14-16, 2012.

"Microassembly through Global Control/Selective Response (GCSR): Controlling Many Robots Through a Single, Global Control Signal." Invited presentation, *20 years of Microrobotics: Progress, Challenges, and Future Directions.* IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS) 2011. San Francisco, CA. September 25, 2011.

Member, Technical Committee on Algorithms for Planning and Control of Robot Motion, IEEE Robotics and Automation Society (2007–2010).[5]

Member, Interational Society for Computational Biology (ISCB).

IEEE Fellows Nominations Committee, IEEE Robotics and Automation Society (March, 2011).

Senior Member, IEEE (2010).

Invited Speaker, Northeastern Structure Symposium (NESS), University of Connecticut, Stoors. October 11, 2008.

Radioactive Materials Authorization, Radiation Safety Division, Occupational and Environmental Safety Office, Duke University. (2007 —   ).

Radiation Safety Training Course for Laboratory Managers (RS-320), Radiation Safety Division, Occupational and Environmental Safety Office, Duke University. July 12, 2007.

Temporary Member, Cell and Molecular Immunology A Study Section (CMIA), National Institutes of Health, Oct. 20-21, 2005.

Reviewer, Special Emphasis Panel on Chronic Fatigue Syndrome (ZRG1 CFS), Center for Scientific Review, National Institutes of Health, Aug. 12, 2005.

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[5]I am not actually sure when this appointment ended.

Invited Speaker, 21st Conference on Uncertainty in Artificial Intelligence (UAI), University of Edinburgh, Scotland. July 29, 2005.

Keynote Speaker, ACM Symposium on Solid and Physical Modeling (SPM05), MIT, June 13, 2005.

Invited speaker, Workshop on Geometry in NMR Protein Structure Determination and NMR Structural Biology, Bellairs Research Institute of McGill University, Holetown, Barbados. Jan. 14–21, 2005.

Program Committee, The Fourth IEEE Computational Systems Bioinformatics Conference (CSB), Stanford CA, August 2005.

Temporary Member, Allergy and Immunology Study Section (ALY), Immunological Sciences Integrated Review Group, National Institutes of Health, Feb. 19-20, 2004.

Plenary lecture, Sixth International Workshop on the Algorithmic Foundations of Robotics (WAFR), Utrecht/Zeist, The Netherlands. July 11-13, 2004

NSF Advisory Panels (1990, 1990, 1991, 1992, 1993, 1994, 1997, 1998, 1999, 2000, 2003).

Temporary Member, Molecular and Cellular Biophysics Study Section (BBCA), Biophysical and Chemical Sciences Integrated Review Group, National Institutes of Health, Oct. 17-18, 2002.

Invited nominator, MacArthur Fellows Program, The John D. and Catherine T. MacArthur Foundation (2001, 2002).

Guest editor, International Journal of Robotics Research, Special Issue on Algorithmic Foundations of Robotics (2001-2002).

Invited speaker, "The New Biology: Technologies for Resolving Macromolecular Communications," An International Symposium Sponsored by the Association of Biomolecular Resource Facilities, Feb. 24–27, 2001 (San Diego).

Invited speaker, EU-NSF Workshop on Motion Planning, Laboratoire d'Analyse et d'Architecture des Systèmes, Centre National de la Recherche Scientifique (LAAS-CNRS), Toulouse, France, June, 2000.

Conference chair, "Fourth International Workshop on the Algorithmic Foundations of Robotics (WAFR 2000)," Dartmouth, March 16-18, 2000.

Invited speaker, "Ninth International Symposium of Robotics Research (ISRR)", Snowbird, Utah (1999).

Invited speaker, "Workshop on Motion Support in Virtual Prototyping," Stanford University, May 5-7, 1999.

Invited speaker, Summer Institute for Cognitive Neuroscience, "Action Systems and Cortical Dynamics," Dartmouth College and Medical School, June 28-July 9 (1999).

Invited speaker, IEEE International Conference on Robotics and Automation, Workshop on Distributed Manipulation (Detroit) May 11, 1999.

Invited speaker, "International Workshop on the Algorithmic Foundations of Robotics (WAFR)," Houston, TX Mar. 5-7, 1998.

Invited speaker, IEEE International Conference on Robotics and Automation, Workshop on Modeling, Contact Analysis, and Simulation of Mechanical Systems in Robotics and Manufacturing, (Belgium, 1998).

NSF Site visitor (1989).

Program Committee, SPIE Microrobotics and Micromanipulation Conference, Intelligent Systems and Advanced Manufacturing Symposium, Boston, (Nov., 1998).

Robotics Program Committee, 15th International Joint Conference on Artificial Intelligence (IJCAI) '97.

Outstanding Reviewer, 15th International Joint Conference on Artificial Intelligence (IJCAI) '97.

Invited Tutorial, "Theoretical Aspects of Sensor Invariants," IEEE/SICE/RSJ International Conference on Multisensor Fusion and Integration for Intelligent Systems. Washington, DC Dec. 8, 1996.

Invited Speaker, IEEE ICRA Workshop on Minimalism in Robot Manipulation (Minneapolis, 1996).

ARPA ISAT Summer Study on Cost-Effective, Capable, and Configurable Multiple Robots (Aug 1996).

Program Committee, "International Workshop on the Algorithmic Foundations of Robotics (WAFR)," Toulouse, France 1996; San Francisco, 1993.

Member, Impact Task Force on Computational Geometry (1994-6).

Invited speaker, *International Symposium on Robotics Research*, (October, 1993).

Associate Editor, IEEE Transactions on Robotics (1988-94).

Guest editor, *Algorithmica*, Vol. 10, Nos. 2/3/4, Aug/Sept/Oct (1993).

Organizing Committee, AAAI 1994, Spring Symposium Series, Stanford University, California Special Sym-

posium on "Detecting and Resolving errors in Manufacturing Systems" March 19-20.

Program Committee, 1st AAAI Fall Symposium on "Sensory Aspects of Robotic Intelligence", Asilomar, CA (Nov, 1991).

Program Committee, IEEE Int. Conf. on Robotics and Automation (ICRA)—(1989, 1993).

American Mathematical Society Short Course, *Mathematical Questions in Robotics*, 96th Meeting of the $\mathcal{AMS}$, (1990)

Invited Speaker, International Symposium on Symbolic and Algebraic Computation, Workshop on Integrated Symbolic-Numeric Computing, July, 1992.

DIMACS Workshop on Algebraic Issues in Geometric Computation (May, 1990).

Organizer, Saratoga Workshop on the Integration of Numerical and Symbolic Computing Methods, Saratoga, NY (July 1990). NSF/AFOSR-Sponsored.

DARPA/ISTO ISAT Summer Study on Autonomous Agents (1991).

9 University Activities

9.1 Duke

University:

Member, Postdoc Compensation Committee, Trinity College of Arts & Sciences (2024–   ).

Member, Standing Committee for Misconduct in Research (SCMR), Duke University and Duke University Medical Center (2019–   ).

Reviewer, Joint School of Medicine/Vice Provost for Research Core Facility Voucher Program (2020).

Author, "Proposal for a Center for Computational Structural Biology and Biomolecular Design", Duke University and Duke University Medical Center, November 28, 2017.

Member, Provost's Advisory Committee on Appointments, Promotions, and Tenure (APT) Committee (9 Semesters total: 9/2008–6/2009, 9/2010–5/2013, and 9/2013–12/2013).

Member, Steering Committee, Deans' Seminars in Theoretical and Computational Neurobiology (2012–2013).

Programs and Affiliations:

Duke Cancer Institute (2022–   ).

Duke Center for Quantitative BioDesign (2022–   ).

Computational Biology and Bioinformatics Ph.D. Program (2006–   ).

Duke Center for Genomic and Computational Biology (GCB) (2017–   ).

Duke Institute for Brain Sciences (DIBS) Faculty, (2008–   ),

Duke Institute for Brain Sciences (DIBS) Investigator, (2008–2012),

Mentor, Duke Scholars in Cardiovascular Medicine, School of Medicine, Duke University (2015-16).

Institute for Genome Sciences and Policy (IGSP), (2006–2014). IGSP was phased out in 2014.

Structural Biology and Biophysics Ph.D. Program (2007–2019).

Cell and Molecular Biology Ph.D. Program (2008–2019).

Computer Science Department:

Executive committee (2006–   ).

Graduate Affairs Committee (2024–   ).

Strategic Planning Committee (2017).

Promotion committee (chair: 2009, 2012, and 2018; member: 2013).

Tenure committees (chair: 2007-8; member: 2006-7, 2010-11, and 2019).

Reappointment committee (member: 2008).

Committee to Write the 10-year Strategic Plan (member: 2009).

CS undergraduate advisor (2014–2017).

Faculty Search Committee (2006-8).
Graduate Admissions Committee (2006-8, 2010-12, 2013-16, 2017–2019, 2020-2023).
Graduate Program Committee (2012-13, 2015-16).
Equipment and Shared Resources Committee (2015-2021).
Communication Committee (2019-2020).
7 RIP ("Research in Progress") Graduate Committees (2006–   ).

Mathematics Department:

Tenure/Promotion committee (member: 2020).

Biochemistry Department, DUMC

Junior faculty mentoring committee (member: 2019–2022).[5]
Appointment/Promotion committee (member: 2013-2014).
Computer and Shared Resources Committee (2006–2011).

Center for Genomic and Computational Biology (GCB):

Tenure committee (member: 2018). Also Department of Biostatistics and Bioinformatics, DUMC.

Cell Biology Department, DUMC.

Junior faculty mentoring committee (member: 2024–   ).

Department of Biostatistics and Bioinformatics, DUMC.

Junior faculty mentoring committee (member: 2024–   ).

Department of Electrical and Computer Engineering and, Department of Biomedical Engineering:

Tenure/Appointment committee (member: 2012).

Department of Biomedical Engineering:

Tenure committee (member: 2022, 2024).

Computational Biology and Bioinformatics (CBB)

Principal Investigator/Project Director (PI/PD), NIH Bioinformatics and Computational Biology Training Program, T32 GM-71340, IGSP, Duke University Medical Center (2007–2010).

CBB Student Advisory Committee (2007–2009).
CBB Executive Committee (2007–2009, 2011–2016, 2017–   ).

Department of Surgery, Duke University Medical Center & Duke Human Vaccine Institute (DHVI):

Junior Faculty Mentoring Committee (member, 2018–2020).[5]

IGSP

Staff/advisor, Duke Genetically-Engineered Machines Team (2007–2009).

9.2   Dartmouth

High-Field NMR Acquisition Committee (2004-5).
Bioinformatics Faculty Search Committee, Departments of Biological Sciences and Computer Science, (2003-4).
Faculty Search Committee, Experimental Physical Chemistry, Chemistry Department (2002-3).
Author, Plan for Bioinformatics and Computational Biology at Dartmouth (2003).
Member, Dartmouth Center for Structural Biology and Computational Chemistry.
Member, Center for Cognitive Neuroscience.
Freshman academic advisor (1998-9, 2004-7).
Faculty Search Committee, Program in Cognitive Neuroscience (1997-8).
Computing & Information Environment Accreditation Committee (CIEAC) (1998-9).
CIEAC Subcommittee on Research Computing (1999).
Committee on Whitaker Foundation Special Opportunity Awards for Biomedical Engineering (1998-9).
Founder, M.D.-Ph.D. Program in Computational Biology (1998–2006).

M.D.-Ph.D. Committee (1999–2006).

Computer Science Department:

   Ph.D. Admissions Committee (2003-2006)
   Chair, Ph.D. Admissions Committee (2004-2006)
   Colloquium Chair (2002-3)
   New Building Committee/Sudikoff Expansion (2002-3).
   Faculty Recruiting Committee (1997-99)
   Curriculum Committee (1997-00)
   Chair, Curriculum Committee 1998, 1999, 2000.
   Computer Equipment Committee (1998-00)
   Department Brochure Committee (1999-00)
   Master's Degree Committee (1997-8)

9.3   Cornell

Director, Cornell Computer Science Robotics Laboratory (1987–91)
Co-director and Co-founder, Cornell Robotics and Vision Laboratory (1991-1997) (with Dan Huttenlocher).
Director, Computer Science Master of Engineering (M.Eng.) Program (1993–1995)
College of Engineering Graduate and Professional Programs Committee (GPPC) (1993–1994)
Chair, Computer Science Master of Engineering Curriculum Committee (1993-1994)
Chair, Computer Science Master of Engineering Admissions Committee (1993-1994)
Engineering Undergraduate Advisor, (1987–1993, 1997)
Computer Science Undergraduate Program Committee, (1992–1994)
COMEPP Faculty Executive Committee, (1987–1990)
Computer Committee, Field of Applied Mathematics, (1990–1994)
Graduate Advisor, Field of Applied Mathematics, (1992–1994)
Recruiting Committee, Department of Computer Science, (1987–1990).

9.3.1   Cornell Field Membership

Computer Science, Applied Mathematics, Cognitive Studies.

10   Teaching

10.1   Duke

"Topics in Computational Biology," Computer Science 590/ CBB 590 (Fall 2013, Spring 2015, Spring 2016, Spring 2018 Spring 2019, Spring 2020, Spring 2021, Spring 2022, Spring 2023).
"Discrete Mathematics for Computer Science," Computer Science 230 (Spring 2014, Fall 2014, Fall 2015, Fall 2017, Fall 2018, Fall 2019, Fall 2020, Fall 2021, Fall 2022).
Biochemistry 593 (every semester, 2016 – 2022).
"Algorithms in Structural Molecular Biology and Biophysics," Computer Science 663/Computational Biology and Bioinformatics 663 (Spring, 2013).
"Topics in Computational Structural Biology," Computer Science 296-02 (2012).
"Algorithms in Drug Design," Computer Science 196.1 (2011).
"Algorithms in Structural Molecular Biology and Biophysics," Computer Science 260/Computational Biology and Bioinformatics 230/Structural Biology and Biophysics 251 (2008).
"Algorithms in Structural Molecular Biology," Computer Science 296/Computational Biology and Bioinformatics 251/Structural Biology and Biophysics 251 (2007, 2009).
Guest lectures: CBB 210, Compsci 300 (2006), Compsci 296 (Robotics) (2007).

10.2   Dartmouth

"Structure and Interpretation of Computer Programs" CS 18 (98,99,2004).
"Computational Molecular Biology" CS 88/188 (2002,2003,2004S,2004F,2006).
"Graduate Artificial Intelligence," CS 104 (99,2000,2003,2004S,2004F,2005).
"Non-Clinical Elective: Research in Computational Biomedicine," MEDI 6042, Dartmouth Medical School (2006).
"Artificial Intelligence" CS 44 (also Cognitive Neuroscience 44) (98).
"3-D Structure in Chemistry and Molecular Biology" CS 88/188 (98).
"Topics in Computational Molecular Biology" CS 88/188 (2000).
"Topics in Computer Animation" CS 88/188 (99).
Guest lectures include: CS 88 (Information Theory), Biology 68 (NMR Section of Molecular Biology), CS 99 (Topics/Senior Culminating Experience), CS 44 (Artificial Intelligence), CS 88 (Bioinformatics).

10.3   Cornell

At Cornell, I usually taught one undergraduate course and one graduate course per year. The courses are numbered (roughly) by level, eg., 1xx=freshman, 2xx=sophomore, etc.

Undergraduate Courses

"Structure and Interpretation of Computer Programs" CS 212 (Honors freshman/sophomore programming course based on Abelson & Sussman's 6.001 at MIT).

Spring 97. Taught using a DYLAN interpreter implemented in JAVA.
Spring 91. Taught using SCHEME.

"Robotics & Machine Vision" CS 462 (92,93).
"Robotics & Machine Vision Laboratory" CS 463 (92, 93).
"Computers and Programming" CS 211. (Sophomore/engineering programming course).

Spring 90. Taught using a SCHEME interpreter implemented in PASCAL.
Fall 87. Taught using PASCAL.

"Artificial Intelligence" CS 472 (1993).
"Artificial Intelligence Laboratory" CS 473 (1993).
"Introduction to Computer Programming" CS100 (Spring 89). (Freshman programming Course).

Graduate Courses

"Robotics" CS 661 (88,89,90,91,92).
"Robotics Laboratory" CS 662 (89,91,93).
"Robot Café" CS 772 or 762 (Spring 88, 90, 91, 92, 93). (Advanced Robotics).
"Dynamic Manipulation and Scientific Computation" CS 761 (Spring 94)
"ProSeminar in Cognitive Studies" CS 770/Psych 522 (Spring 88)
"Seminar on Artificial Intelligence" CS 779. (Fall 87, Spring 88)

11   Selected Lectures and Colloquia

"Probabilistic Structural Biology: The Challenge of Determining, Describing and Predicting the Structure of a Flexible Protein" (with T. Oas). CASP-16,[6] Punta Cuna, Dominican Republic (December 4, 2024).

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[6]CASP (Critical Assessment of Structure Prediction) is a biennial community experiment to determine the state of the art in modeling protein structure. Participants are provided with amino acid sequences of target proteins, and build models of the corresponding three-dimensional structures.

"Structure of a Two-Domain Protein with a Flexible Linker: Assessment and Evaluation of 39 Entries to CASP 16." CASP-16[6] Assessors & Organizers Meeting. Hotel Odelya, Missionsstrasse 21, 4051 Basel, Switzerland (September 28, 2024).

"CS and AI are Revolutionizing Drug Discovery and Health Care." Best of Duke Talk, Duke/Duke Kunshan University (March 21, 2024).

"Structure of a Two-Domain Protein with a Flexible Linker: A Continuous Distribution of Interdomain Orientation Derived from NMR Residual Dipolar Couplings." CASP-16[6] Special Interest Group on Modeling Ensembles and Alternative Conformations of Proteins (March 7, 2024).

"Computational Protein Design, Anti-(microbial | cancer | viral) Resistance." TriPoD (Triangle Protein Design) Group, North Carolina (November 2, 2023).

"Few-shot Protein Design Predictions: Biologics, Resistance Mutations, and Machine Learning" Duke Center for Quatitative BioDesign (November 11, 2022).

"*In silico* design of V2-apex antibodies yields improved HIV-1 breadth and potency by improving non-conserved side-chain interactions" (with G. Holt). Joint HIV-1 Meeting, Vaccine Research Center, NIAID, NIH. (March 21, 2022).

"Computational Protein Design: Peptide Inhibitors, PPI Design, and Targeted Biologics (antibodies)" (Invited Talk). Predictive Reagent Antibody Replacement Technology (PRe-ART) Symposium. Universität Bayreuth. Bayreuth, Germany (September 18, 2019).

"Some Geometric and Computational Challenges Arising in Structural Molecular Biology" (Invited Talk). 35th International Symposium on Computational Geometry (SoCG 2019), Portland, OR. June 21, 2019.

"Some Mathematical and computational challenges arising in structural molecular biology."
    Given at:

    Applied Math and Analysis Seminar, Duke University. May 2, 2019.
    TTIC Colloquium, Toyota Technological Institute (TTIC) at the University of Chicago. Chicago, IL. April 23, 2018.

"Computational Protein Design, with Applications to Predicting Resistance Mutations, and HIV."
    Given at:

    Computer Science Department, Johns Hopkins University. November 20, 2018.
    Structural Biology Discussion Group Seminar, Genetic Medicine Building, University of North Carolina at Chapel Hill. September 20, 2018.
    Molecular Biology and Biophysics Seminar, Uconn Health, University of Connecticut, Farmington, CT. April 25, 2017.
    Keynote talk, Structural Bioinformatics and Computational Biophysics (3DSIG), ISMB Satellite Meeting, Orlando, Fl. July 8, 2016.
    Invited talk, 2nd Protein Engineering Canada (PEC) Conference, Ottawa, ON. June 18, 2016.
    Colloquium. Computer Science and Chemistry Departments, Indiana University, Bloomington, IL. September 25, 2015.
    Keynote talk, Computer Science Research Symposium, Dartmouth College, May 8, 2015.

"Redefining Structure: New Approaches for (1) Deep Topological Sampling of Protein Structures, and (2) Continuous Probability Density Function for Biomolecular Interdomain Orientations." Invited talk, Experimental NMR Conference (ENC). Pittsburgh, PA. April 12, 2016.

"Big Data Analytics for Global Health." IBM, Morrisville NC. November 14, 2014.

"Computational Protein Interface Design, Cystic Fibrosis, and HIV."
    Given at:

    Department of Chemistry, Duke University. March 4, 2014.
    Department of Biology, MIT, Cambridge MA. December 11, 2013.
    Biophysics Lecture Series, California Institute of Technology, Pasadena, CA. February 11, 2013.

"Designing Proteins Using Computer Algorithms." Department of Physics, University of North Carolina. October 22, 2013.

"Computational Protein Design, With Applications to Cystic Fibrosis and HIV." Computer Science Department Distinguished Lecture. Tulane University. April 12, 2013.

"Protein Interface Design, Cystic Fibrosis, and HIV."
  Given at:

    Computational Biology and Bioinformatics (CBB) Seminar, September 17, 2012.
    and
    Keynote talk, Tenth International Workshop on the Algorithmic Foundations of Robotics (WAFR),
      CSAIL, MIT, Cambridge MA. June 13, 2012.

"The Compass that Steered Robotics." Symposium for Dexter Kozen, Computer Science Department,
  Cornell University, April 26, 2012.
"Computational Redesign of a Broadly Neutralizing Antibody." Vaccine Research Center, NIAID, NIH,
  Bethesda, MD, May 3, 2011.
"HIV-1 Pan-neutralization through Antibody Redesign." NIH Director's Pioneer Award Finalist Presenta-
  tion, Bethesda, MD, May 2, 2011.
"Anticipating Resistance."
  Given at:

    The Institute for Computational Engineering and Sciences (ICES) Seminar – Molecular Biophysics
      Series, University of Texas at Austin, February 28, 2011.
    Department of Bioinformatics and Genomics, University of North Carolina at Charlotte, October 22,
      2010.
    MIT Computer Science and Artificial Intelligence Laboratory (CSAIL), March 5, 2010.

"Algorithms for Protein Design and Drug Design."
  Given at:

    Computer Science Department, University of British Columbia, Vancouver. April 1, 2011.
    Northeastern Structure Symposium (NESS), University of Connecticut, Stoors. October 11, 2008.
    Computer Science Department, Cornell University, September 18, 2008.
    Algorithms Seminar, Computer Science Department, Duke University, September 8, 2008.

"Automated NOE Assignment and Protein Structure Determination using Residual Dipolar Couplings."
  Triangle Magnetic Resonance Seminar (TRIMR), National Institute for Environmental Health Sciences
  (NIEHS), National Institutes of Health (NIH), Research Triangle Park, NC. December 2, 2009.
"Will Resistance Be Futile?" Structural Biology and Biophysics Retreat, Duke University Medical Center,
  May 16, 2009.
"Computational Protein Design and Drug Design."
  Given at:

    Biochemistry and Biophysics Seminar, School of Medicine, University of North Carolina, Chapel Hill.
      November 18, 2008.
    Department of Biochemistry, Duke University Medical Center. November 20, 2008.

"Algorithms for Protein Structure Determination by NMR," Algorithms Seminar, Computer Science De-
  partment, Duke University, October 15, 2007.
"Solution Structures of Native and Denatured Proteins Using Residual Dipolar Couplings."
  Given at:

    Department of Biochemistry, The Research Institute at The Hospital for Sick Children, University of
      Toronto, October 23, 2007.
    Structural Biology and Biophysics Seminar, Duke University Medical Center, Jan. 22, 2007.

"Building Very Small Mobile Micro Robots."
  Given at:

    Inaugural Lecture, Nanotechnology Public Lecture Series, MIT (Research Laboratory for Electronics,
      EECS, and Microsystems Technology Laboratories). April 19, 2007.
    Department of Computer Science, University of Toronto. October 22, 2007.
    Visualization Forum, Duke University. September 28, 2007.

"The Nonribosomal Code: Natural (& Unnatural) Products from the Biosphere's Microbial Drug Factories,"
  Institute for Genome Sciences and Policy, Duke University, Feb. 1, 2007.

"A Steerable, Untethered, 250×60 μm MEMS Mobile Micro-Robot." Given at:

Department of Mechanical Engineering and Material Science, Duke University, November 20, 2006.
MIT Computer Science and Artificial Intelligence Laboratory (CSAIL), April 24, 2006.
Dartmouth Physics Department Colloquium, October 7, 2005.

"Algorithmic Challenges in Structural Molecular Biology and Proteomics." Given at:

Biochemistry Department, School of Medicine, Duke University, February 16, 2006.
Computer Science Department, Carnegie-Mellon University, September 21, 2005.
Computational Biology Department, University of Pittsburgh Medical School, September 20, 2005.
Computer Science Department, Rensselaer Polytechnic Institute, September 12, 2005.
Invited Lecture, 21$^{\text{st}}$ Conference on Uncertainty in Artificial Intelligence (UAI), University of Edinburgh, Scotland. July 29, 2005.
Keynote Lecture, ACM Symposium on Solid and Physical Modeling (SPM05), MIT, June 13, 2005.
Pathology Research and Review Seminar, Dartmouth-Hitchcock Medical Center, May 10, 2005.
Computer Science Department, University of Maryland, May 3, 2005.
Computer Science Department, Duke University, April 11, 2005.
Electrical Engineering Department, University of Washington, Seattle. February 10, 2005.
Biomedical Engineering Department, University of Michigan, Ann Arbor. January 27, 2005.
Computer Science Department, University of Chicago. November 10, 2004.
Plenary lecture, Sixth International Workshop on the Algorithmic Foundations of Robotics (WAFR), Utrecht/Zeist, The Netherlands. July 11, 2004,
Dartmouth Computer Science Department, July 7, 2004,
Computer Science Department, Tufts University, April 13, 2004, and
MIT Computer Science and Artificial Intelligence Laboratory (CSAIL), Feb. 19, 2004.

Workshop on Geometry in NMR Protein Structure Determination and NMR Structural Biology, Bellairs Research Institute of McGill University, Holetown, Barbados. Three talks:

"Computational Challenges in NMR Structural Genomics," January 14, 2005.
"An Expectation/Maximization Nuclear Vector Replacement Algorithm for Automated NMR Resonance Assignments," January 14, 2005.
"Automated Assignment and Protein Structure from Sparse, Unassigned NMR Data," January 15, 2005.

"Protein Geometry and its Role in Structural Molecular Biology and Proteomics," Meeting of the American Mathematical Society (AMS), Lawrenceville, New Jersey, April 17-18, 2004.

"An Expectation/Maximization Nuclear Vector Replacement Algorithm for Automated NMR Resonance Assignments," Harvard Medical School, November 20, 2003.

"Computational Biochemistry," Foley Inaugural Lecture, Dartmouth College, October 8, 2003.

"MEMS Algorithms and Systems for Massively-Parallel Distributed Manipulation," GRASP Lab, Department of Computer Science, University of Pennsylvania, April 25, 2003.

"Algorithmic Challenges in Structural Genomics," Penn Bioinformatics Forum, University of Pennsylvania, April 24, 2003.

"Computational Challenges in NMR Structural Genomics," Dartmouth Physics Department Colloquium, May 24, 2002.

"Algorithmic Challenges in Structural Molecular Biology," Robert Mueller-Thuns Distinguished Lecture in Computer Science, at the University of Illinois (Urbana-Champaign), March 11-12, 2002.

"Algorithmic Challenges in Structural Molecular Biology," Triangle Distinguished Lecture in Computer Science, University of North Carolina at Chapel Hill, Duke, and N.C. State, Feb. 18-19, 2002.

"Use of Multiple Conformations to Model Protein Flexibility in Core-Binding Factor," Department of Biochemistry, Dartmouth Medical School, March 4, 2002.

"Algorithms and Systems for High-Throughput NMR Structural Molecular Biology," Harvard University, Division of Engineering and Applied Sciences, December 14, 2001.

"Algorithms and Systems for High-Throughput Structural Molecular Biology," Sandia National Labs, March 15, 2001.

"Algorithms and Systems for High-Throughput Structural Molecular Biology," at *The New Biology: Technologies for Resolving Macromolecular Communications,* An International Symposium Sponsored by the Association of Biomolecular Resource Facilities, Feb. 25, 2001 (San Diego).

"MEMS Algorithms and Systems for Massively-Parallel Distributed Manipulation," Middlebury College, November 14, 2000.

"Algorithms for High-Throughput Structural Molecular Biology," The Rowland Institute for Science, Cambridge, MA, October 25, 2000.

"MEMS Algorithms and Systems for Massively-Parallel Distributed Manipulation," Department of Mechanical Engineering, University of Michigan, September 29, 2000.

"Algorithms for Structural Molecular Biology" Harvard Medical School, September 19, 2000.

"Motion Planning Opportunities in Haptics and Structural Biology," EU-NSF Workshop on Motion Planning, Laboratoire d'Analyse et d'Architecture des Systèmes, Centre National de la Recherche Scientifique (LAAS-CNRS), Toulouse, France, June, 2000.

"MEMS Algorithms and Systems for Massively-Parallel Distributed Manipulation," NSF Planning Meeting, Ninth International Symposium on Robotics Research, Snowbird, Utah, October 10, 1999.

"Algorithmic MEMS," Visualization Center Colloquium, Computer Science Department, Purdue University, April 22, 1998.

"Algorithmic Foundations for Planar MEMS Force-Field Devices: Geometric Algorithms for Massively-Parallel Distributed Manipulation," National Science Foundation, Washington, DC, June 10, 1997.

"Robotics & Microelectromechanical (MEM) Systems: Massively-Parallel Systems for Distributed Manipulation at a Micro Scale," Crump Institute for Biomedical Imaging, Department of Molecular and Medical Pharmacology, UCLA. March 25, 1997.

"Algorithmic Foundations for Planar Force-Field Devices: Geometric Algorithms for Massively-Parallel Distributed Manipulation," Computer Science Department Colloquium, Washington University, St. Louis, January 15, 1997.

"Massively-Parallel Distributed Manipulation," Artificial Intelligence Laboratory, MIT, October 2, 1996.

"Geometric Algorithms for Massively-Parallel Distributed Manipulation," given at:

Computer Science Department, New York University, November 1, 1996.
Algorithms Seminar, Computer Science Department, Stanford University, October 17, 1996.
Computer Science Department, Dartmouth College, October 3, 1996.
Division of Engineering and Applied Sciences, Harvard University, September 29, 1996.
Computer Science Department, Brown University, September 27, 1996.
Department of Industrial Engineering and Operations Research, U. C. Berkeley, September 9, 1996.

"Algorithmic Foundations for Planar Force-Field Devices: Geometric Algorithms for Massively-Parallel Distributed Manipulation," Robotics Laboratory, Computer Science Department, Stanford University, September 20, 1996.

"Massively-Parallel Distributed Manipulation," Department of Engineering, Brown University, September 26, 1996.

"Massively-Parallel Distributed Manipulation," Manipulation Laboratory, Robotics Institute, Carnegie-Mellon University. July 25, 1996.

"Towards Ubiquitous, Distributed Manipulation: Teams of Mobile Robots and Arrays of Microelectromechanical Silicon Cilia," Interval Research Corporation, Palo Alto, CA (May, 1996).

"Massively-Parallel Algorithms for Micro-manipulation," Computer Science Department Colloquium, Princeton University, Princeton, NJ (April, 1996).

"Towards Ubiquitous, Distributed Manipulation." Given at:

University of Washington, Computer Science Department, (March, 1996).
Duke University, Computer Science Department, (March, 1996).
Duke University, ECE Department, (March, 1996).
Computer Science Department Colloquium, Princeton University, Princeton, NJ (December, 1995).
Robotics Institute Colloquium, Robotics Institute, Carnegie-Mellon University, Pittsburgh, PA (December, 1995).

"Distributed Manipulation Using Mobile Robots and MEMS," UCLA Computer Science Colloquium, Los Angeles, CA (1995).

"Distributed Manipulation Using Massively Parallel Micro-fabricated Actuator Arrays," Berkeley Engineering Systems Colloquium, U. C. Berkeley, Berkeley, CA (1995).

"Small and Large: Distributed Robotic Manipulation," Computer Science Department, University of British Columbia, Vancouver. March 1995.

"Model-based Geometric Algorithms for Animation and Multimedia," Interval Research, Palo Alto, CA Feb. 1995.

"Large and Small: Distributed Robotic Manipulation," SRI, Menlo Park, CA Dec. 1994.

"Sensorless Manipulation Using Massively Parallel Micro-fabricated Actuator Arrays," Xerox PARC, Palo Alto, CA, Dec. 1994.

"Distributed Robotic Manipulation, Large or Small," Computer Science Department, Dartmouth College, Nov. 1994.

"Distributed Robotic Manipulation, Large and Small," Computer Science Department, U. C. Berkeley, Nov. 1994.

"Distributed Robotic Manipulation," Robotics Laboratory, Computer Science Department, Stanford University, Oct. 1994.

"Programmable Part-Feeders, Large and Small", Wright-Patterson Air Force Base, Dayton, Ohio, May, 1994.

"On the Information Content of Distributed Manipulation Protocols for Cooperating Autonomous Mobile Robots," International Workshop on the Algorithmic Foundations of Robotics (WAFR), San Francisco, Feb. 1993.

"A Theory of Manipulation and Control for Microfabricated Actuator Arrays," National Science Foundation, Oct. 21, 1993.

"Manipulation and Control of Microfabricated Actuator Arrays," Air Force Office of Sponsored Research, Oct. 22, 1993.

"Geometric Algorithms for Design and Analysis of Dynamic Microelectromechanical Structures," AFOSR Electronic Prototyping Grantees Review Meeting, University of Michigan, Ann Arbor MI. May 26, 1993.

"Design of Dynamic Microelectromechanical Structures," Workshop On Geometric Algorithms For Manufacturing, IEEE Int. Conf. on Robotics and Automation, May 2, 1993.

"On Information Invariants in Robotics," AAAI Workshop on Computational Theories of Interaction and Agency, University of Chicago, Feb 20-21, 1993.

"Map Making and Localization for Mobile Robots using Shape Metrics," AAAI Fall Symposium Series, (with Russell Brown). *Application of Artificial Intelligence to Real-World Autonomous Mobile Robots*; October 23-25, 1992. Cambridge, Massachusetts.

"Geometric Algorithms, Rational Rotations, and Computational Topology," International Symposium on Symbolic and Algebraic Computation, Workshop on Integrated Symbolic-Numeric Computing, Berkeley, CA. Thursday, July 30, 1992. (Invited).

"On Computing the Homology Type of a Triangulation (part I)," Computer Science Department, University of Illinois at Urbana-Champaign, July 16, 1992.

"On Computing the Homology Type of a Triangulation (part II): A Probabilistic Analysis of Sparse SNF (Smith Normal Form) Computation," (with David Chang) Computer Science Department, University of Illinois at Urbana-Champaign, July 17, 1992.

"A Lennonist Perspective on Autonomous Agents, or, Nothing Can Be Seen That Isn't Shown," 1st AAAI Fall Symposium on Sensory Aspects of Robotic Intelligence, Asilomar, CA (Nov, 1991).

"Geometric Theories of Robot Motion Planning with Uncertainty and Dynamics," Computer Science Colloquium, Stanford University, May 1991.

"Dynamics, Uncertainty, and Performance Measures in Robot Motion Planning", Computer Science Department, University of Chicago, April, 1991.

"Compliance, Uncertainty, Dynamics, and Time-Optimality in Robot Motion Planning", Courant Institute and Computer Science Department, New York University, Nov. 1990.

"Geometrical Theories of Robot Motion Planning with Uncertainty, Compliance, Dynamics, and Time-

Optimality", Robotics Institute and Computer Science Department, Carnegie-Mellon University, Nov. 1990.

"Uncertainty, Compliance, Dynamics, and Time-Optimality in Robot Motion Planning", Computer Science Department, Princeton University, 1990.

"Planning Collision-Free Paths and Near Time-Optimal Trajectories in Cluttered Environments", United Parcel Service Research and Development, Danbury, CT October, 1990.

"Provably-Good Approximation Algorithms for Gross-Motion Planning and Optimal-Time Trajectory Planning", Yale University, October, 1990.

"Simulation, Planning, and the Motion of Compliantly-Connected Rigid Bodies in Contact: A System for Analyzing Designs for Assembly" Saratoga Workshop on the Integration of Numerical and Symbolic Computing Methods, Saratoga, NY (July 1990).

"On The Motion of Compliantly-Connected Rigid Bodies in Contact: A System for Analyzing Designs for Assembly", Xerox Palo Alto Research Center, June 29, 1990.

"Geometric Reasoning and Planning," Xerox Palo Alto Research Center, June 28, 1990.

"Motion Planning and Configuration Space," Xerox Palo Alto Research Center, June 27, 1990.

"Advances in Robotics and Automation Through Computational Geometry", Wright-Patterson Air Force Base, Dayton, Ohio, June, 1990.

"Planning and Executing Robot Assembly Strategies in the Presence of Uncertainty", American Mathematical Society Short Course, *Mathematical Questions in Robotics*, Louisville, Kentucky. January 16-17, 1990

"Provably Good Approximation Algorithms for Optimal Kinodynamic Planning", AT&T Bell Labs, Murray Hill, N.J., Dec, 1989.

"A Provably Good Approximation Algorithm for Optimal-Time Trajectory Planning", Department of Information Engineering, Oxford University, England, August 1989.

"Motion Planning and Configuration Space," I.R.S.T (Istituto per la Richercha Scientifica e Technologica), Istituto Trentino di Cultura, Trento, Italy. July 21 and 24, 1989.

"Motion Planning with Uncertainty", I.R.S.T., July 25, 1989.

"Error Detection and Recovery", I.R.S.T., July 26, 1989.

"Polynomial-Time Approximation Schemes for Optimal-Time Trajectory Planning", I.R.S.T., July 27, 1989.

"A Provably Good Approximation Algorithm for Optimal-Time Trajectory Planning", Carnegie-Mellon Robotics Institute, July, 1989.

"A Provably Good Approximation Algorithm for Optimal-Time Trajectory Planning", Northwestern University, Dept. of Mechanical Engineering, May, 1989.

"Kinodynamic Planning: (A Provably Good Approximation Algorithm for Optimal-Time Trajectory Planning)", MIT Artificial Intelligence Lab, March, 1989.

"Error Detection and Recovery for Robot Motion Planning with Uncertainty", Robotics Laboratory, Stanford University. Feb. 1989.

"Error Detection and Recovery in Robotics," Panel on Robot Autonomy and Dexterity, NASA Conference on Space Telerobotics, Jet Propulsion Laboratory, California Institute of Technology, Jan. 1989.

"Error Detection and Recovery for Robot Motion Planning with Uncertainty". Computer Science Department, Duke University, Feb. 1988.

"Error Detection and Recovery for Robot Motion Planning with Uncertainty". Computer Science Division, U. C. Berkeley, Dec. 1987.

"Motion Planning with Uncertainty" Courant Institute Geometry Seminar, NYU, Oct. 1987

"Thoughts on Error Detection and Recovery" US/France Workshop on Automatic Robot Programming, MIT, April, 1987.

"Error Detection and Recovery for Robot Motion Planning with Uncertainty". Given at:

Computer Science Department and Robotics Institute, Carnegie-Mellon University, April, 1987.
Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, April, 1987.
Computer Science Department, Cornell University, April, 1987.
Division of Engineering and Applied Sciences, Harvard University, April, 1987.
Computer Science Department, University of Wisconsin at Madison, March, 1987.
Computer Science Department, University of Southern California, March, 1987.

California Institute of Technology, January, 1987.

"Robot Motion Planning with Uncertainty in the Geometric Models of the Robot and Environment: A Formal Framework for Error Detection and Recovery", IBM Watson Research Center, Yorktown, NY, 1986.

12 Students and Post-Docs Supervised

12.1 Thesis Advisor (Ph.D)

1. Patrick G. Xavier, *Provably-Good Approximation Algorithms for Optimal Kinodynamic Robot Plans*, PhD (April, 1992) Computer Science Department, Cornell University.
Nominated by Cornell Computer Science Department for the ACM Distinguished Dissertation Award.
Dr. Xavier was a Senior Member of the Technical Staff at Sandia National Labs (1992-2019).

2. Amy Briggs, *Efficient Geometric Algorithms for Robot Sensing and Control.* PhD (August, 1994) Computer Science Department, Cornell University.
Dr. Briggs is now a full Professor of Mathematics and Computer Science (with tenure) at Middlebury College.

3. Russell Brown, *Localization, Mapmaking, and Distributed Manipulation with Flexible, Robust Mobile Robots.* PhD (February 1995) Computer Science Department, Cornell University.
First (post-Ph.D.) job: Dr. Brown was a Senior Member of the Technical Staff at Sandia National Labs.

4. Karl F. Böhringer. *Programmable Force Fields for Distributed Manipulation, and their Implementation Using Micro-fabricated Actuator Arrays.* Ph.D. (August 1997) Computer Science Department, Cornell University.
Nominated by Cornell Computer Science Deptartment for the ACM Distinguished Dissertation Award.
Dr. Böhringer is now John M. Fluke Distinguished Chair of Engineering at the University of Washington (U.W.), Seattle, and director of the U.W. MEMS Laboratory.

5. James Jennings, *Distributed Manipulation for Mobile Robots.* Ph.D. (May 1998) Computer Science Department, Cornell University.
First job: Assistant Professor of EECS at Tulane University.
Dr. Jennings is now a professsor at NC State University.

6. Chris Langmead, *Molecular Replacement for Nuclear Magnetic Resonance: Application to NMR Resonance Assignment and Protein Structure Determination.* Ph.D. (2004) Computer Science Department, Dartmouth College.
Dr. Langmead is now an Associate Professor of Computer Science at Carnegie-Mellon University.

7. Ryan Lilien (Ph.D., 2004) is listed in §12.1.1.

8. Craig McGray *Design, Fabrication, Control, and Programming of MEMS Micro-Robots.* (Ph.D., 2005). Computer Science Department, Dartmouth College.
Dr. McGray is now a researcher at the MicroElectroMechanical Systems (MEMS) Project, Semiconductor Electronics Division, Electronics and Electrical Engineering Laboratory, National Institute of Standards and Technology (NIST).

9. Igor Paprotny, *Design, Fabrication and Parallel Control of Distributed Systems of Stress-engineered MEMS Microrobots for Microassembly.* Ph.D. (2008) Computer Science Department, Dartmouth College.
First job: postdoc at the Berkeley Sensor and Actuator Center (BSAC), U. C. Berkeley.
Second job: Dr. Paprotny was a research faculty member at The Berkeley Sensors and Actuator Center (BSAC), U.C. Berkeley.
He is currently an Associate Professor (with tenure) at the University of Illinois.

10. Anthony K. Yan, *Geometric Methods for NMR Structure Determination of Symmetric Homo-oligomers,* Ph.D. (2008) Computer Science Department, Dartmouth College.
First Job: Dr. Yan was a postdoc in the laboratory of Dr. Pei Zhou, Duke Biochemistry Department.

11. Ivelin Georgiev, *Novel Algorithms for Computational Protein Design, with Applications to Enzyme Redesign and Small-Molecule Inhibitor Design*, Ph.D. (2009) Computer Science Department, Duke

University.
Outstanding Ph.D. Dissertation Award, Computer Science Department, Duke University (2009).
First job: computational biologist in the Structural Biology Section of the Vaccine Research Center, National Institute for Allergy and Infectious Diseases (NIAID).
Dr. Georgiev was co-head of the Structural Bioinformatics Section at the Vaccine Research Center, NIAID, NIH.
Dr. Georgiev is now an Associate Professor (with tenure) at Vanderbilt University Medical Center.

12. Faisal Reza, *Computational Molecular Engineering of Nucleic Acid Binding Proteins and Enzymes*, Ph.D. (2010) Department of Biomedical Engineering and Program in Computational Biology and Bioinformatics, Duke University.
Dr. Reza was a postdoc in the laboratory of Peter M. Glazer, Department of Therapeutic Radiology, Yale University School of Medicine.
He is currently Team Lead, CDC Vaccine Team, Vaccine Task Force (TF), 2019 Novel Coronavirus Response, and TitleTeam Co-Lead, Tiberius CDC Data Science & Analytics Team, 2019 Novel Coronavirus Response. Canters for Disease Control (CDC).

13. Michael Zeng, *Novel Algorithms for Automated NMR Assignment and Protein Structure Determination*, Ph.D. (2011) Department of Computer Science, Duke University.
Dr. Zeng is an associate professor (with tenure) at Tshingua University (IIIS) starting 9/2012.

14. Chittaranjan (Chittu) Tripathy, *Novel Algorithms for Protein Structure Determination from Sparse NMR Data*, Ph.D. (2012) Department of Computer Science, Duke University.
First job: Dr. Tripathy was teaching faculty at Duke University starting 6/2012.
He is now Distinguished Data Scientist at Walmart Labs.

15. Inho Yoon, *Developing In Vivo Intracellular Neuronal Recording System for Freely-Behaving Small Animals,* Ph.D. (2013) Department of Electrical and Computer Engineering, Pratt School of Engineering, Duke University.
Dr. Yoon is now a researcher at Intel.

16. Cheng-Yu Chen, *Studies on Redesign and Solution Structure Determination of Nonribosomal Peptide Synthetases and Redox Regulation of Phosphatase*, Ph.D. (2013) Department of Biochemistry, School of Medicine, Duke University Medical Center.
First job: Dr. Chen was a post-doc in the lab of James Prestegard, University of Georgia.
He is now Senior Scientist at Bristol Myers Squibb, Cambridge.

17. Jeffrey Martin, *Geometric Algorithms for Protein Structure Determination Using Measurements From NMR Spectroscopy*, Department of Computer Science, Duke University. Ph.D. (2014).
Outstanding Dissertation Award, Computer Science Department, Duke University.
Nominated by Duke Computer Science Department for the ACM Distinguished Dissertation Award.
First job: Dr. Martin was a researcher at SCALGO Scalable Algorithmics, LLC.
Currently CEO and Founder at Cuchaz Interactive, LLC.

18. Kyle Roberts, *Novel Computational Protein Design Algorithms with Applications to Cystic Fibrosis and HIV*, Program in Computational Biology & Bioinformatics, Duke University, Ph.D. (2014).
First job: Dr. Roberts is now a protein design scientist at Arzeda, Inc.

19. John MacMaster, *Solution-Phase Nuclear Magnetic Resonance Studies of a Nonribosomal Peptide Synthetase Adenylation Domain, of a Bacterial Glycosyltransferase, and the Rational Design of Inhibitors and Mutants of Glycosyltlransferases*, Department of Computer Science, Duke University. Ph.D. (2015).

20. Swati Jain, *RNA 3D Structure Analysis and Validation, and Design Algorithms for Proteins and RNA*, Program in Computational Biology & Bioinformatics, Duke University. Ph.D. (2015).
First job: Dr. Jain is now a postdoc in the laboratory of Tamar Schlick, NYU Medical School.
Currently she is senior developer at Ten63 Therapeutics, Inc.

21. Pablo Gainza, *Computational Protein Design with Ensembles, Flexibility and Mathematical Guarantees, and its Application to Drug Resistance Prediction, and Antibody Design*, Department of Computer Science, Duke University. Ph.D. (2015).
First job: Dr. Gainza was a research associate (postdoc), and then a Scientist, in the Laboratory of Protein Design and Immunoengineering, EPFL, Lausanne, Switzerland.
Currently: Senior Scientist, Monte Rosa Therapeutics. Basel, Switzerland.

22. Mark Hallen, *Protein and drug design algorithms using improved biophysical modeling*, Department of Computer Science, Duke University. Ph.D. (2016).
First job: Dr. Hallen was an Assistant Professor at Toyota Technological Institute, University of Chicago (TTIC).
He is currently CTO, Ten63 Therapeutics, Inc..

23. Adegoke Ojewole, *Efficient New Computational Protein Design Algorithms, with Applications to Drug Resistance Prediction and HIV Antibody Design* , Program in Computational Biology & Bioinformatics, Duke University. Ph.D. (2018).
First job: Dr. Ojewole was a Vertex Fellow at Vertex Pharmaceuticals.
Second job: He was next Senior Software Engineer and AI Scientist (Early Clinical Development), Genentech, San Francisco.
Currently: Senior Manager, BioPharma AI/ML, NVIDIA Corp.

24. Jonathan Dragon Jou, *Novel Computational Protein Design Algorithms with Sparse Residue Interaction Graphs, Ensembles, and Mathematical Guarantees, and their Application to Antibody Design*, Department of Computer Science, Duke University. Ph.D. (2018).
Dr. Jou is currently a scientist and senior developer at Schrödinger.

25. Anna Lowegard, *Novel Algorithms and Tools for Computational Protein Design with Applications to Drug Resistance Prediction, Antibody Design, Peptide Inhibitor Design, and Protein Stability Prediction*, Program in Computational Biology & Bioinformatics, Duke University. Ph.D. (2019).
First job: Dr. Lowegard was Computational Antibody Engineer at GlaxoSmithKline (GSK), London UK
Second job: Senior Computational Biologist, Research Bio Engineer in BioAI, InstaDeep Ltd, London, UK.
Dr. Lowegard is currently Senior Molecular Data Scientist in Biologics at Novo Nordisk.

26. Marcel Frenkel, *Combined computational, experimental, and assay-development studies of protein:protein and protein:small molecule complexes, with applications to the inhibition of enzymes and protein:protein interactions*, Department of Biochemistry, School of Medicine, Duke University Medical Center. Ph.D. (2019).
Dr. Frenkel is currently CEO, Ten63 Therapeutics, Inc..

27. Siyu Wang, *Computational Protein Design with Non-proteinogenic Amino Acids and Small Molecule Ligands, with Applications to Protein-protein Interaction Inhibitors, Anti-microbial Enzyme Inhibitors, and Antibody Design*, Program in Computational Biology & Bioinformatics, Duke University. Ph.D. (2021).

28. Grahm Holt, *Ensemble-based Computational Protein Design: Algorithms and Applications*, Program in Computational Biology & Bioinformatics, Duke University. Ph.D. (2022).
Dr. Holt is currently a senior scientist at VantAI, a subsidiary of Roivant.

29. Kelly Huynh, *Discovery and Characterization of Novel Thanatin Orthologs Against* Escherichia coli *LptA and* Pseudomonas aeruginosa *LptH*, Department of Biochemistry, School of Medicine, Duke University Medical Center. Ph.D. (2023).
Dr. Huynh is currently a senior protein scientist at Generation Bio.

30. Nathan Guerin, *New Computational Methods to Predict Cancer Resistance Mutations and Design D-Peptide Therapeutics*, Department of Computer Science, Duke University. Ph.D. (2023).
Outstanding Ph.D. Dissertation Award, Computer Science Department, Duke University.
Dr. Guerin is currently Director of Engineering at Ten63 Therapeutics, Inc..

12.1.1 Thesis Advisor, M.D.-Ph.D

Ryan Lilien, *Novel Algorithms for Structural Molecular Biology and Proteomics.* Ph.D. (2004) Computer Science Department, Dartmouth College. M.D. (2006) Dartmouth Medical School.
Dr. Lilien is currently an assistant professor of computer science and medicine at the University of Toronto, and CSO at Cadre Research Labs.

12.2 Post-Docs Supervised

1. Dinesh Pai (1988-91). (First Job: Assistant Professor of Computer Science at U.B.C. Now a Full Professor of Computer Science at U.B.C.)
2. Jonathan Rees (1991-92). (First job: Sussex/MIT. Now lead scientist at Millennium Pharmaceuticals on the pathways database project).
3. Daniela Rus (1992-94). (First job: Assistant Professor of Computer Science at Dartmouth. Now a full Professor of Computer Science at the MIT EECS Department). John D. and Catherine T. MacArthur Fellow (2002-2007).
4. John J. Kelley III (1999–2001). (Now at the University of Michigan).
5. Christopher Bailey-Kellogg (1999–2001). (First Job: Assistant Professor of Computer Science at Purdue. Now full Professor of Computer Science at Dartmouth).
6. Lincong Wang (2001-2006). (First job: senior scientist at Boehringer Ingelheim Pharmaceuticals. Now a full Professor at the Joint Center for Systems Biology of Jilin University and the University of Georgia, and College of Computer Science and Technology, Jilin University, Changchun, Jilin, P. R. China).
7. Ram Mettu (2002–2005). (First job: Assistant Professor of Electrical and Computer Engineering at the University of Massachusetts, Amherst.
Now Associate Professor (with tenure) at the Department of Computer Science, Tulane University).
8. Rahul Ray (2004-2006). (First job: Assistant Professor of Computer Science at IIT-Madras).
9. Ryan Lilien (2004-2006) is listed in §12.1.1.
10. Serkan Apaydin (2004–2008)
First job: Faculty of Engineering and Sciences at Sabanci University in Istanbul, Turkey. He is now a professor at Izmir Institute of Technology, Turkey.
11. Nanjiang Shu (2008–2009)
Now at Boston University.
12. Anna Yershova (2008–2011).
Now at the University of Illinois at Urbana-Champaign.
13. Michael Zeng (2011–2012)
Dr. Zeng is an Associate professor (with tenure) at Tshingua University (IIIS).
14. Stuart Endo-Streeter (2009–2013)
Now a research scientist at UNC.
15. Chittaranjan (Chittu) Tripathy (2012–2013)
First job: Dr. Tripathy was teaching faculty at Duke University starting 6/2012.
He is now Principal Data Scientist at Walmart Labs.
16. Kyle Roberts (2014–2015)
First job: Dr. Roberts is now a protein design research scientist at Arzeda, Inc.
17. Pablo Gainza (2015).
First job: Dr. Gainza was a research associate (postdoc), and then a Scientist, in the Laboratory of Protein Design and Immunoengineering, EPFL, Lausanne, Switzerland.
Currently: Senior Scientist, Monte Rosa Therapeutics. Basel, Switzerland.
18. Mark Hallen (2016).
First job: Dr. Hallen was an Assistant Professor at Toyota Technological Institute, University of Chicago (TTIC).
He is currently CTO, Ten63 Therapeutics, Inc..
19. Jonathan Dragon Jou (2018–2020). Dr. Jou is currently a scientist and senior developer at Schrödinger.
20. Anna Lowegard, (2019).
First job: Dr. Lowegard is currently Computational Antibody Engineer at GlaxoSmithKline (GSK), London UK
Currently: Senior Computational Biologist, Research Bio Engineer in BioAI, InstaDeep Ltd, London, UK.
21. Jeffrey Martin (2016–2018, 2020-2022).
First job: Dr. Martin was a researcher at SCALGO Scalable Algorithmics, LLC.
Currently CEO and Founder at Cuchaz Interactive, LLC.

22. Kelly Huynh (2023).
23. Grahm Holt (2022–23).
24. George "Bert" Cortina M.D., Ph.D. Research fellow (Donald Lab, CS) and resident (house staff) Anæsthesiology (2023–   ).
25. Allen McBride (2024-   ).

12.3   Thesis/Project Advisor, M.S. and Master of Engineering

Marius Moscovici, *Mobile Robot Control System* (M.Eng., Electrical Engineering 1989)

Bob Blondell, *Design of a microprocessor driven generic controller for a mobile robot base* (M.Eng., Electrical Engineering 1990)

Steve Shollenberger, *Design of a microprocessor driven generic controller for a mobile robot base* (M.Eng., Electrical Engineering 1990)

Bill Ford, *The Design of an Infrared Proximity Detector System and the Redesign of the Cornell Generic Controller for a Mobile Robot*, (M.Eng., Electrical Engineering 1991)

Pete Chady, CHRISTENE: *A Computer Vision Ball Tracker for Real Time Robotics Applications* (M.Eng., Computer Science 1993)

Anthony K. Yan, *Color Differentiation for Motion Capture*, (M.Eng., Computer Science) (1998).

Haoning Fu, *An Algorithm For Determining Backbone Structures of Protein Turns and Loops Using Multiple Residual Dipolar Couplings in Two Media* (M.S., Computer Science, 2004).

Jeffrey Martin, *Algorithms for Structure Determination of Symmetric Proteins from Nuclear Magnetic Resonance Data*, Computer Science Department, Duke University, (M.S., 2009).
Outstanding M.S. Thesis Award, Computer Science Department, Duke University (2009).

Yang Qi, *On Provable Algorithms for Determination of Continuous Protein Interdomain Motions from Residual Dipolar Couplings.* Department of Biochemistry and Department of Computer Science, Duke University. M.S. in Computer Science (2016).

12.4   Senior Theses Supervised (Selected List)

Susanna Leng (Dartmouth '98) Honors thesis, "Data-Directed Conformational Search: Using Global Optimization to Determine Large Protein Structure from Sparse NMR Data."

Alik Widge (Dartmouth '99) Honors thesis, "A Method for Automatic Determination of Protein Secondary Structure from Sparse Unassigned NMR Data." Winner, John G. Kemeny Computing Prize (First Prize).
Alik went on to complete an M.D.-Ph.D. at CMU.

Ryan McCullough (Dartmouth '99) Senior project, "Algorithms and Systems for the Prediction of Metal-DNA Binding."

Tim Danford (Dartmouth '01) Senior Thesis, "Cleavage-Based Algorithms for Experiment Planning and Data Analysis in Stable Isotope Assisted Structural Mass Spectrometry."
Tim went on to complete a Ph.D. in Computer Science, working with David Gifford at MIT.

Hunter Nisonoff, Senior thesis: *Efficient Partition Function Estimation in Computational Protein Design: Probabilistic Guarantees and Characterization of a Novel Algorithm*, Department of Mathematics, Duke University, B.S. (2015). Graduation with High Honors. Co-advised with Mauro Maggioni.

Francois Thelot, Senior thesis: *A maximum entropy-based approach for the description of the conformational ensemble of calmodulin from paramagnetic NMR*, Department of Mathematics, Duke University, B.S. (2016). Graduation with Honors.

David Zhou, Senior thesis: *Computational Design of RNA with Perturbations*, Department of Computer Science, Duke University, B.S. (2017). Graduation with High Distinction.

Aditya Mukund, Senior thesis: *Partition function estimation in computational protein design with continuous-label Markov Random Fields*, Department of Computer Science, Duke University, B.S. (2017). Graduation with Highest Distinction.

Caleb Watson, Senior thesis: *Incorporation of Non-proteinogenic Amino Acids (ncAAs) into* OSPREY *Protein Redesign Framework*, Department of Computer Science, Duke University, B.S. (2023). Graduation with High Distinction.

Jaden (Yuxi) Long, Senior thesis: *Predicting Affinity Through Homology (PATH): Interpretable Binding Affinity Prediction with Persistent Homology*, Departments of Computer Science and Mathematics, Duke University, B.S. (2024). Graduation with Highest Distinction.

12.5   Advisor, Undergraduate Research (Selected List)

Jaden Long, CS, Duke University (2022-23).

Tyler Nisonoff, CS, Duke University (2014).

Francois Thelot, Physics, Duke University (2013–2015)..

Nina Sun, HHMI Fellow, Duke University (2014).

David Zhou, CS, Duke University (2014).

Jonathan Jou, Computer Science, Duke University (2008).
Currently a Ph.D. Student, Computer Science, Duke University.

Nick Patrick, Computer Science, Duke University (2007–2008).
Winner of Goldwater Scholarship in science, mathematics and engineering for the 2008-09 academic year.

Mohini (Mona) Sridharan, Computer Science and Chemistry, Dartmouth College (1998–1999).
Mona went on to complete a Ph.D. in Molecular Biology and Biophysics at UCSF.

12.6   Thesis Reader: PhD (Selected List)

Completed Ph.D.

Klara Kedem (Tel-Aviv University), *Problems in Planning Collision Free Motion for A Rigid Robot System in the Plane: Theory and Application*, PhD. 1988.

Doug Ierardi (CS) *On the Complexity of Quantifier Elimination in the Theory of Algebraically Closed Fields*, PhD. 1989.

Jong-Hun Lee (Civil and Environmental Engineering), *A Spectral-Textural Classifier for Digital Imagery*, PhD. 1990.

Kenjiro Takai Miura (Mechanical Engineering), C^2 *Gregory Patch and Its Applications to Computer-Aided Geometric Design*, PhD. 1991.

Eric Wynters (Applied Mathematics) *Optimal Motion Planning for Multiple Point Robots in the Plane*, PhD. 1991.

David Baraff (CS [graphics]), *Dynamic Simulation of Non-penetrating Rigid Bodies*, PhD. 1992.

Peter Wayner (CS), *Using Algebraic Invariants and Grouping to Speed Object Recognition in a Single, Two-Dimensional Image*, PhD. 1992.

Vivek Bhatt (Mechanical Engineering), *Three Dimensional Frictional Rigid Body Impacts*, PhD. 1995.

Ronen Brafman (Stanford) *Qualitative Models of Information and Decision Making: Foundations and Applications,* PhD, 1996.

Jed Lengyel, (CS [graphics]) *Three-Dimensional Reconstruction and Rendering of Moving Coronary Arteries,* PhD 1996.

Rama Prasad (Mechanical Engineering) *Investigation of Friction in SCREAM-Fabricated Micro-Electro Mechanical Systems,* PhD 1997.

Yan-Bin Jia, (CS) Robotics Institute, CMU, *Geometric Computation and Dynamic Observations of Pose and Motion*, PhD 1998.

Keith Kotay, (CS) Dartmouth, *Self-reconfigurable Robot Systems.*

Zack Butler, (CS) CMU *Cooperative Coverage in Unknown Highly-Structured Environments*, Ph.D. 2000.

P. David Hauck (Mechanical Engineering).

Robert Freimer (CS).

Christine Piatko (CS).

Paul Wanuga (Computer Graphics)

Steve Fontes, (Mechanical Engineering)

Alin Popescu, Ph.D. 2004 Computer Science Department, Dartmouth College.

Rob Fitch, Ph.D. 2004 Computer Science Department, Dartmouth College.

Olga Vitek, Ph.D. 2005 Statistics Department, Purdue University. *An Inferential Approach to Protein Backbone Nuclear Magnetic Resonance Assignment.*

Shobha Potluri, Ph.D. 2007, Computer Science Department, Dartmouth College.

Xiaoduan Ye, Ph.D. 2007, Computer Science Department, Dartmouth College.

Alex Miklos, Department of Biochemistry, Duke University Medical Center. (2008)

Raluca Gordan, Department of Computer Science, Duke University. (2009)

Urmi Majumder, Department of Computer Science, Duke University.

Vincent Chen, Department of Biochemistry, Duke University Medical Center.

Dan Keedy, Department of Biochemistry, Duke University Medical Center. (2012)

Amber Harold, Department of Chemistry, Duke University.

Charlie Cooper, Department of Biochemistry, Duke University.

Yang Qi, Department of Biochemistry, Duke University.

Atul Kaushik Rangadurai, Department of Biochemistry, Duke University.

Manon Ruffini, Mathématiques et Informatique Appliqués de Toulouse, L'Université de Toulouse 3 Paul Sabatier.

Yuze Hou, Department of Biochemistry, Duke University.

Yingfan Wang, Department of Computer Science, Duke University.

12.7 Thesis Reader: MS (Selected List)

Richard Eaton Cornell (Computer Graphics), *Explicit Geometric Constraints*, M.S. 1988.

Mark Reichert Cornell (Computer Graphics), *A Two-Pass Radiosity Method Driven by Lights And Viewer Position*, M.S. 1992.

Samuel Stearns, Dartmouth *A Progressive Folding Algorithm for RNA Secondary Structure Prediction,* (M.S., Computer Science) 2003.

13 Research Grants and Contracts

13.1 Selected Funded Grants

(2022-2027) R35 GM-144042, National Institutes of Health, National Institute of General Medical Sciences (NIGMS). "Computational and Experimental Studies of Protein Structure and Design." Established Investigator R35 MIRA Award. $3,194,742 (total):

> **(2023-2025)** Equipment Supplement, "Supplement for Purchase of a GPU-enabled Computer Cluster," 3R01 GM-144042-02S2, $179,940.
>
> **(2022-2025)** Research Supplement to Promote Diversity in Health-Related Research, 3R35 GM-144042-01S1, $159,810.
>
> **(2022-2027)** *Computational and Experimental Studies of Protein Structure and Design.* Parent grant and Initial application 1R35 GM-144042-01, $2,854,992.

(2022-2023) TRPC4 Antagonist with Losartan Block Marfan Aortopathy. The Marfan Foundation (with J. Turek, J. Nellis, and H. Dietz).

(2008-2022) R01 GM-078031, National Institutes of Health, National Institute of General Medical Sciences (NIGMS), $4,305,505 (total):

> **(2018-2019)** Equipment Supplement, "Supplement for Purchase of a FortéBio Octet RED96e Bio-Layer Interferometry (BLI) System", 3R01 GM-078031-09S1, $232,298.
>
> **(2018-2022)** *Computational Structure-Based Protein Design*, Competing renewal, 2R01 GM-078031-09, $1,403,624.
>
> **(2015-2018)** Research Supplement to Promote Diversity in Health-Related Research, 3R01 GM-078031-06S1, $145,619.
>
> **(2014-2018)** *Computational Structure-Based Protein Design*, Competing renewal, 2R01 GM-078031-05, $1,263,794.
>
> **(2008-2014)** *Computational Active-Site Redesign and Binding Prediction via Molecular Ensembles*, Initial application 1R01 GM-078031, $1,211,813.

(2017-2022) R01 GM-118543, *Deep Topological Sampling of Protein Structures.* National Institutes of Health, National Institute of General Medical Sciences (NIGMS), $1,386,317 (total):

> **(2019-2021)** Equipment Supplement, "Supplement for Purchase of a GPU-enabled Computer Cluster," 3R01 GM118543-03S1, $170,613.
>
> **(2017-2021)** 1R01 GM-118543, $1,215,704.

(2012–2014) *Miniature Microdrive for Intracellular Recordings in Freely Behaving Mice* (with R. Mooney). R21 NS-79929. National Institutes of Health, National Institute of Neurological Disorders and Stroke (NINDS), and National Institute of Biomedical Imaging and Bioengineering (NIBIB), $382,256.

(2011–2015) *Novel Receptor-Ligand Interactions in Glomerulonephritis* (with M. Foster). R01 DK-88904. National Institutes of Health, National Institute of Diabetes and Digestive and Kidney Diseases (NIDDK), $1,392,232.

(2011–2013) *Development of Methods to Quantify Biological and Pathological Aging of Cartilage* (with V. Kraus). R21 AG-3978. National Institutes of Health, National Institute on Aging (NIA), $225,295.

(2011–2016) *IGERT: Training Program in Wireless Intelligent Sensor Networks* (with S. Ferarri, P. Agarwal, and R. Parr). National Science Foundation, DGE-1068871. $3,126,326.

(2010–2012) *Replacement Equipment Components for an 800 MHz NMR Spectrometer.* NIH S10 Shared Instrumentation Program, (with L. Spicer). Direct Costs: $441,700

(2008-2010) *Multi-wall Carbon Nanotubes and MEMS Microrobots for Intracellular Neuronal Recordings*, Duke Institute for Brain Science, (with R. Mooney and G. Finkelstein). $150,000.

(2002-2012) *Automated NMR Assignment and Protein Structure Determination*, National Institutes of Health, National Institute of General Medical Sciences (NIGMS) (R01 GM-65982) $2,683,997 (total):

> **(2009-2011)** ARRA Supplement, 3R01 GM-65982-08S1, $262,516.
>
> **(2007-2012)** Competing renewal 2R01 GM-65982, $1,209,668.
>
> **(2002-2007)** Initial application 1R01 GM-65982, $1,211,813. NIGMS Protein Structure Initiative.

(2005-2010) *Bioinformatics and Computational Biology Training Program.* National Institutes of Health, National Institute of General Medical Sciences (T32 GM-71340), $1,079,891 (total).

> **(2005-2010)** Initial application 1T32 GM-71340, $899,175. Tom Kepler, PI, 2005–2007. B. Donald, PI, 2007-2010.
> **(2009-2010)** ARRA Supplement, 3T32 GM-71340-05S1, $180,716. (PI: B. Donald).

(2003-2008) *Design of* C. parvum *and* T. gondii *DHFR-TS (Dihydrofolate reductase-thymidylate synthase) Inhibitors*, (with A. Anderson), National Institutes of Health, National Institute of General Medical Sciences (NIH/NIGMS) and NIAID, (R01 GM-067542) $1,440,000.

(2004) *An Institute for Computational Science at Dartmouth* (with M. Gazzaniga and J. Barucha). Role: Faculty Director. The Neukom Family Foundation. $22,000,000.

(2003-2005) "Algorithmic Challenges in Computational Biology," the National Science Foundation, $75,000.

(2000-2006) *Microelectromechanical Systems for Infosecurity*, the Institute for Security Technology Studies, Office for Domestic Preparedness, U.S. Department of Homeland Security (DHS), $1,160,196.

(2001-2002) John Simon Guggenheim Memorial Fellowship, *Algorithms for Structural Proteomics: New Frontiers in Physical Geometric Algorithms,* $35,000.

(2001-2003) *Physical Geometric Algorithms and Systems for High-Throughput NMR Structural Biology,* the National Science Foundation, $66,000.

(2001-2003) *Physical Geometric Algorithms and Systems for Structural Biology using Mass Spectrometry,* the National Science Foundation, $66,000.

(1999–2002) *MEMS Algorithms and Systems for Distributed Manipulation*, the National Science Foundation, $369,000, plus $17,000 in REU supplements.

(1999–2002) Microsoft Research, Microsoft Corporation, *Workstations for an Instructional Laboratory in Psychological and Brain Sciences*, Program in Cognitive Neuroscience, (Equipment donation) approx. $100,000.

(1999-2002) Microsoft Research, Microsoft Corporation, *Workstations for Graduate Student Research*, Computer Science Department (Equipment donation) $450,000.

(1999-2001) *Challenges in Micro-Manipulation: Massively Parallel MEMS Algorithms and Systems,* National Science Foundation, $66,000.

(1998-2000) *MEMS and Microrobotics,* National Science Foundation, $66,000.

(1998-2003) National Science Foundation, *Systems Science for Physical Geometric Algorithms,* CISE Research Infrastructure Grant, (with D. Nicol, D. Rockmore, and D. Kotz), $1,300,901.

(1997–2000) *Planning and Control for Massively Parallel Manipulation,* NSF Challenges in Computer and Information Science and Engineering, (with K. Goldberg, J. Canny, and L. Kavraki). $1,434,000.

(1999–2001) *Research Instrumentation for Distributed Reconfigurable Robot Systems*, (with D. Rus) National Science Foundation, $120,000.

1996—99 National Science Foundation, *Distributed Manipulation Algorithms using Massively-Parallel Microfabricated Actuator Arrays.* (with N. C. MacDonald). $360,000, plus $24,000 in REU supplements.

1993—96 National Science Foundation. *Task-Level Planning and Task-Directed Sensing for Robots in Uncertain Environments.* $234,000.

1994 ARPA/National Science Foundation (SGER), *A Computational Approach to the Design of Dynamic Microelectromechanical Structures*, $50,000.

1989—94 National Science Foundation Presidential Young Investigator (PYI) Award. $25,000 per year, plus $37,500 in matching funds. Total $312,500.

1991-1994 Air Force Office of Sponsored Research, *Applications of geometric algorithms to machining, manufacturing, and design.* Dan Huttenlocher, Paul Chew, and Joe Mitchell are co-PI's. Approx. $550,000.

1992-5 Air Force Office of Sponsored Research, *Applications of geometric algorithms to machining, manufacturing, and design (AASERT Supplement).* Dan Huttenlocher is co-PI. Approx. $120,000.

1990—93 National Science Foundation ILI Program, *Development of an Undergraduate Laboratory Curriculum in Robotics*, $100,000, with $100,000 matching funds from the Cornell School of Engineering.

1993-94 Sandia National Laboratories, funding for graduate research assistants. Approximately $60,000.

1992 National Science Foundation, CISE Program. *Research in Mobile Autonomous Robotic Motion, Sensing, and Planning in Unstructured Environments: A Proposal for a Mobile Robot Equipped with a Vision System.* Dan Huttenlocher and Carlo Tomasi are co-PI's. Approx. $30,000.

1990–92 National Science Foundation, *New Algorithmic Techniques for Task-level Robot Planning*, $131,317.

July, 1990 National Science Foundation and AFOSR, *A Workshop on the Integration of Numerical and Symbolic Computing Methods*, $28,000. Joe Mundy and Deepak Kapur are co-PI's.

1989–90 AT&T Bell Laboratories. *Research in Mobile Autonomous Robotic Motion, Sensing, and Planning in Unstructured Environments*, $50,000.

1991-2 AT&T Bell Labs *Development of an Undergraduate Laboratory Curriculum in Robotics*, $10,000, Dan Huttenlocher is co-PI.

Jul. 1989–Jun. 1990 *Kinodynamic Motion Planning*. Mathematical Sciences Institute. $24,000.

Jul. 1988–Jun. 1990 *Towards Task-Level Robot Programming*, National Science Foundation IRI-8802390. $133,571.

1992 Intel Corp. *Design, Real-Time Control, Fabrication, and Programming of Advanced Robotic Devices*, approx. $16,400 (equipment).

1991 Intel Corp. *Design, Real-Time Control, Fabrication, and Programming of Advanced Robotic Devices*, $143,000 (equipment).

1990 Intel Corp. *Design, Real-Time Control, Fabrication, and Programming of Advanced Robotic Devices*, $62,961 (equipment).

Jan. 1988–May 1989 *Planning and Simulation of Robot Manipulation Strategies*, Mathematical Sciences Institute. Principal Investigators: John Hopcroft, Bruce Donald. $59,838.

(1985-88) *Error Diagnosis and Recovery in Task-Level Robot Planning.* NASA/Jet Propulsion Laboratory (JPL) Graduate Student Researcher Fellowship. Jet Propulsion Laboratory, California Institute of Technology, Oak Grove Drive, Pasadena, CA. $52,500.

14   List of Publications

14.1   Books

1. *Algorithms in Structural Molecular Biology*, MIT Press (Cambridge: 2011), 464 pp.
2. *Algorithmic and Computational Robotics: New Directions*, (with K. Lynch and D. Rus) A. K. Peters (Boston: 2001), 408 pp.
3. *Symbolic and Numerical Computation for Artificial Intelligence*, Academic Press, Harcourt Brace Jovanovich, (London: 1992) (with D. Kapur and J. Mundy). 369 pp.
4. *Robotics*, Symposia in Applied Mathematics, vol 41. American Mathematical Society Press, Providence, RI (1990) (with Baillieul, Brockett, *et al.*). 196 pp.
5. *Error Detection and Recovery in Robotics*, Lecture Notes in Computer Science, Vol. 336, Springer-Verlag, New York (1989). 314 pp.

14.2   Papers in Refereed Journals

14.2.1   Cover Articles

Journal papers # 36, 12, 17, 23, 29, 33, and 57 below are cover articles.

14.2.2   Structural Molecular Biology and Biochemistry

6. "Improved HIV-1 Neutralization Breadth and Potency of V2-Apex Antibodies by *In Silico* Design" (with G. Holt, J. Gorman, S. Wang, A. Lowegard, B. Liu, T. Lin, B. Zhang, M. Louder, M. Frenkel, K. McKee, S. Rawi, O'Dell R., C.-H. Shen, N. Doria-Rose, and P. Kwong) *Cell Reports* 2023; 42(**7**): 112711.
7. "Discovery, characterization, and redesign of potent antimicrobial thanatin orthologs from *Chinavia ubica* and *Murgantia histrionica* targeting *E. coli* LptA" (with K. Huynh, A. Kibrom and P. Zhou). *Journal of Structural Biology: X.* 2023; (**8**): 100091. https://doi.org/10.1016/j.yjsbx.2023.100091
8. "Novel, provable algorithms for efficient ensemble-based computational protein design and their application to the redesign of the c-Raf-RBD:kRas protein-protein interface" (with A. Lowegard, M. Frenkel, G. Holt, J. Jou, and A. Ojewole). *PLoS Computational Biology* 2020; 16(**6**):e1007447. doi: 10.1371/journal.pcbi.1007447.
9. "Computational Analysis of Energy Landscapes Reveals Dynamic Features that Contribute to Binding of Inhibitors to CFTR-Associated Ligand" (with G. Holt, J. Jou, N. Gill, A. Lowegard, J. Martin, and D. Madden). *Journal of Physical Chemistry B.* 2019; 123(**49**):10441–10455.
10. "Toward Broad Spectrum DHFR inhibitors Targeting Trimethoprim Resistant Enzymes Identified in Clinical Isolates of Methicillin-Resistant *Staphylococcus aureus*" (with S. Reeve, D. Si, J. Krucinska, Y. Yan, K. Viswanathan, S. Wang, G. Holt, M. Frenkel, A. Ojewole, A. Estrada, S. Agabiti, J. Alverson, N. Gibson, N. Priestly, A. Wiemer, and D. Wright). *ACS Infectious Diseases* 2019; 5(**11**):1896–1906.
11. "Continuous interdomain orientation distributions reveal components of binding thermodynamics," (with Y. Qi, J. Martin, A. Barb, F. Thélot, A. Yan, and T. Oas). *Journal of Molecular Biology* 2018; 430(**18** Pt B): 3412–3426.
12. "OSPREY 3.0: Open-Source Protein Redesign for You, with Powerful New Features" (with M. Hallen, J. Martin, A. Ojewole, J. Jou, A. Lowegard, M. Frenkel, P. Gainza, H. Nisonoff, A. Mukund, S. Wang, G. Holt, D. Zhou, and E. Dowd). *Journal of Computational Chemistry* 2018; 39(**30**): 2494–2507. Cover article.

13. "OSPREY Predicts Resistance Mutations using Positive and Negative Computational Protein Design" (with A. Ojewole, A. Lowegard, P. Gainza, S. Reeve, I. Georgiev, and A. Anderson). *Methods in Molecular Biology, Methods Mol Biol.* 2017;1529:291-306. In: Vol. 1529 (Computational Protein Design). Springer-Verlag: Berlin (2016). ISBN 978-1-4939-6635-6

14. "Algorithms for protein design" (with P. Gainza and H. Nisonoff). *Current Opinion in Structural Biology* 2016; **(39)**:160-26. doi: 10.1016/j.sbi.2016.03.006.

15. "Crystal structure, conformational fixation and entry-related interactions of mature ligand-free HIV-1 Env" (with Do Kwon Y, Pancera M, Acharya P, Georgiev IS, Crooks ET, Gorman J, Joyce MG, Guttman M, Ma X, Narpala S, Soto C, Terry DS, Yang Y, Zhou T, Ahlsen G, Bailer RT, Chambers M, Chuang GY, Doria-Rose NA, Druz A, Hallen MA, Harned A, Kirys T, Louder MK, O'Dell S, Ofek G, Osawa K, Prabhakaran M, Sastry M, Stewart-Jones GB, Stuckey J, Thomas PV, Tittley T, Williams C, Zhang B, Zhao H, Zhou Z, Lee LK, Zolla-Pazner S, Baxa U, Schon A, Freire E, Shapiro L, Lee KK, Arthos J, Munro JB, Blanchard SC, Mothes W, Binley JM, McDermott AB, Mascola JR, and Kwong PD). *Nature Structural & Molecular Biology* 2015; 22**(7)**: 522–31.

16. "Protein Design Algorithms Predict Viable Resistance to an Experimental Antifolate" (with S. Reeve, P. Gainza, K. Frey, I. Georgiev, and A. Anderson). *Proceedings of the National Academy of Sciences, U.S.A. (PNAS)* 2015; 112**(3)**:749–754.

17. "Systematic solution to homoöligomeric structures determined by NMR" (with J. Martin and P. Zhou). *Proteins: Structure, Function, and Bioinformatics* 2015; 83**(4)**:651–661. Cover Article.

18. "Enhanced potency of a broadly neutralizing HIV-1 antibody *in vitro* improves protection against lentiviral infection *in vivo*" (with R. Rudicell, Y. Kwon, S.Y. Ko, A. Pegu, M. Louder, I. Georgiev, X. Wu, J. Zhu, J. Boyington, X. Chen, W. Shi, Z. Yang, N. Doria-Rose, K. McKee, S. O'Dell, S. Schmidt, G.Y. Chuang, A. Druz, C. Soto, Y. Yang, B. Zhang, T. Zhou, J.P. Todd, K. Lloyd, J. Eudailey, K. Roberts, R. Bailer, J. Ledgerwood, NISC Comparative Sequencing Program, J. Mullikin, L. Shapiro, R. Koup, B. Graham, M. Nason, M. Connors, B. Haynes, S. Rao, M. Roederer, P. Kwong, J. Mascola, and G. Nabel). *Journal of Virology* 2014; 88**(21)**:12669–82.

19. "Structure of an HIV-1 Neutralizing Antibody Target: A Lipid Bound gp41 Envelope Membrane Proximal Region Trimer" (with P. Reardon, H. Sage, S. Dennison, J. Martin, S. Alam, B. Haynes, and L. Spicer). *Proceedings of the National Academy of Sciences, U.S.A. (PNAS)* 2014; 111**(4)**:1391-6.

20. "OSPREY: Protein Design with Ensembles, Flexibility, and Provable Algorithms" (with P. Gainza, K. Roberts, I. Georgiev, R. Lilien, D. Keedy, C.-Y. Chen, F. Reza, A. Anderson, D. Richardson, and J. S. Richardson). *Methods in Enzymology* 2013; **(523):**87-107.

21. "Design of Epitope-Specific Probes for Sera Analysis and Antibody Isolation" (with I. Georgiev, P. Acharya, S. Schmidt, Y. Li, D. Wycuff, G. Ofek, N. Doria-Rose, T. Luongo, Y, Yang, T. Zhou, J. Mascola, P. Kwong). *Retrovirology* 2012; **9**(Suppl. 2):P50.

22. "HASH: a Program to Accurately Predict Protein H$^\alpha$ Shifts from Neighboring Backbone Shifts" (with J. Zeng, and P. Zhou). *Journal of Biomolecular NMR* 2013; 55**(1)**:105-118.

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14.2.6 Microelectromechanical Systems (MEMS) and Nanoscience

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14.2.7 Robotics and Motion Planning

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99. "Minimalism, Distribution, and Supermodularity," (with J. Jennings and D. Rus) *Journal of Experimental and Theoretical Artificial Intelligence (JETAI).* Special issue on Software Architectures for Hardware Agents; Vol. 9 No. 2-3 (1997) pp. 293–321.

100. "Information Invariants for Distributed Manipulation", (with J. Jennings and D. Rus) *International Journal of Robotics Research*, Vol. 16, No. 5 (1997). pp. 673-702.

101. "Information Invariants in Robotics," *Artificial Intelligence*, Vol. 72, Nos. 1–2, **pp. 217–304** (Jan. 1995).

102. "Provably Good Approximation Algorithms for Optimal Kinodynamic Planning for Cartesian Robots and Open Chain Manipulators" (with P. Xavier) *Algorithmica*, **(14),** No. 6 (1995), pp. 443-479.

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14.2.8   Computational Geometry

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14.3   Selected Protein Structures

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  *For a list of all protein stuctures (*circa *29) reported in our papers, please visit:*
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14.4   Patents and Patent Applications

125. *Novel antibodies for HIV and methods of making and using the same* WO2024097957A1 WIPO (PCT) Patent Application (2023).

126. *Compositions for inhibiting KRas signaling and methods of making and using same* (with A. Lowegard and M. Frenkel). U.S. Patent US 12024725-B2 issued July 2, 2024.

127. *Thanatin Peptide Compositions and Methods of Making and Using Same* (with K. Huynh and P. Zhou). U.S. Patent Patent Application, Attorney Docket No. DU8031P, Application No. 63/449,372, filed on March 2, 2023.

128. *Novel Antibodies For HIV and Methods of Making and Using Same.* U.S. Patent Patent Application filed, Atty Docket No. DU7794PROV (2022).

129. *Compositions for inhibiting KRas signaling and methods of making and using same* (with A. Lowegard and M. Frenkel). U.S. Provisional Patent 62/030,975 filed May 28, 2020.

130. *Carbon Nanotube Probe* (with I. Yoon, I. Borzenets, K. Hamaguchi, R. Mooney, and G. Finkelstein), U.S. Patent Pending, PTO Provisional Patent #61/711,511, filed October 9, 2012: 22 claims.

131. *Compositions and methods for inhibiting the interaction between CFTR and CAL* (with P. Cushing, P. Boisguerin, R. Volkmer, L. Vouilleme, K. Roberts, and D. Madden). U.S. Patent application, US 2013/006005 A1. (March 7, 2013).

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133. *System for Image Manipulation and Animation Using Embedded Constraint Graphics* (with J. T. Ngo), U.S. Patent #5,933,150, issued August 3, 1999: 91 claims.

14.5   Other Invention Disclosures

134. *Reagent for inhibiting KRas signaling* (with A. Lowegard and M. Frenkel). Invention Disclosure T-006815, Office of Licensing & Ventures, Duke University & Medical Center (2019).

135. *Computational Design of a Novel Modular Antibody-Conjugated Entry and Replication Inhibitor (MAC-ERI) for Prophylactic and Therapeutic Treatment of Zika Virus* (with M. Frenkel). Invention Disclosure 557, Office of Licensing & Ventures, Duke University & Medical Center (2016).

14.6   Papers in Refereed Conferences

Note: In both Computer Science and Computational Biology, certain conferences are highly selective and rigorously refereed, often by 3 reviewers plus the conference chairs. Conference papers are published not as one-page abstracts, but as 8-12 page full papers (in 10pt double-column format). For this reason, conference papers are considered primary publications in the field.
Selectivity can be roughly quantitated by the acceptance rate.

14.6.1 Computational Molecular Biology

A. Algorithms in Structural Molecular Biology

136. DexDesign: a new OSPREY-based algorithm for designing *de novo* D-peptide inhibitors (with N. Guerin, H. Childs, and P. Zhou) *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Boston. (April 29–May 2, 2024). Acceptance rate: less than $\frac{58}{352}$. In *Lecture Notes in Computer Science* 14758, Springer (Cham, Schweizerische Eidgenossenschaft) pp. 336–249.

137. Discovery, characterization, and redesign of potent antimicrobial thanatin orthologs from *Chinavia ubica* and *Murgantia histrionica* targeting *E. coli* LptA (with K. Huynh, A. Kibrom, and P. Zhou). American Society for Biochemistry and Molecular Biology, Discover BMB Conference, Seattle, WA. March, 2023. *Journal of Biological Chemistry* 2023; 299:(**3**):S640.

138. Non-canonical inhibitors target the CAL binding site: new approaches to stabilize functional ΔF508-CFTR (with N. Gill, J. Amacher, P. Cushing, Y. Zhao, L. Wallace, A. Pletnev, M. Spaller, S. Cullati, S. Gerber, P. Boisguerin, D. Casalena, D. Auld, S. Wang, and D. Madden). 2023 European Cystic Fibrosis Society Conference. Dubrovnik, Croatia. March 29–April 1, 2023.

139. resistor: An algorithm for predicting resistance mutations using Pareto optimization over multistate protein design and mutational signatures (with N. Guerin and T. Kaserer). *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, San Diego. (May 22-25, 2022). In *Research in Computational Molecular Biology, RECOMB 2022,* Lecture Notes in Computer Science, vol. 13278. Springer (Cham, Schweizerische Eidgenossenschaft). pp. 387–389.

140. "Minimization-Aware Recursive K* (MARK*): A Novel, Provable Algorithm that Accelerates Ensemble-based Protein Design and Provably Approximates the Energy Landscape" (with J. Jou, G. Holt, and A. Lowegard). *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Washington, DC. (May 5-8, 2018). Springer Nature Switzerland AG (2019) RECOMB 2019, Lecture Notes in Bioinformatics (LNBI) 11467, pp. 101-–119.

141. "cats (Coordinates of Atoms by Taylor Series): Protein design with backbone flexibility in all locally feasible directions" (with M. Hallen). *Proc. International Conference on Intelligent Systems for Molecular Biology (ISMB)*, Prague (July, 2017).

142. "*BBK** (Branch and Bound over *K**): A Provable and Efficient Ensemble-Based Algorithm to Optimize Stability and Binding Affinity over Large Sequence Spaces" (with A. Ojewole, J. Jou, and V. Fowler). *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Hong Kong. (May 3-7, 2017). Acceptance rate: less than $\frac{38}{180}$. In *Research in Computational Molecular Biology,* Lecture Notes in Computer Science (LNCS), Springer-Verlag (Berlin) vol. 10229, pp. 157–172.

143. "lute (Local Unpruned Tuple Expansion): Accurate continuously flexible protein design with general energy functions and rigid-rotamer-like efficiency" (with M. Hallen and J. Jou). *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Los Angeles, CA. April, 2016. Acceptance rate: less than $\frac{35}{170}$. In *Research in Computational Molecular Biology,* Lecture Notes in Bioinformatics (LNBI), Springer-Verlag (Berlin), Volume 9649, 2016, pp. 122–136.

144. "comets (Constrained Optimization of Multistate Energies by Tree Search): A provable and efficient algorithm to optimize binding affinity and specificity with respect to sequence" (with M. Hallen). *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Warsaw, April 12-15, 2015. Acceptance rate less than $\frac{36}{170}$. In *Research in Computational Molecular Biology Lecture Notes in Computer Science*, Springer-Verlag (Berlin), Volume 9029, 2015, pp. 122–135.

145. "BWM*: A Novel, Provable, Ensemble-based Dynamic Programming Algorithm for Sparse Approximations of Computational Protein Design" (with J. Jou, S. Jain, and I. Georgiev). *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Warsaw, April 12-15, 2015. Acceptance rate less than $\frac{36}{170}$. In *Research in Computational Molecular Biology Lecture Notes in Computer Science*, Springer-Verlag (Berlin), Volume 9029, 2015, pp. 154–166.

146. "Visualizing the Inter-Domain Motions of a Pathogenic Protein using Sparse RDC Data," (with

Y. Qi, J. Martin, A. Yan., F. Thelot, and T. Oas) *Biophysical Journal* 2015; 108**(2)**:58a. DOI:http://dx.doi.org/10.1016/j.bpj.2014.11.353

147. "An Efficient Parallel Algorithm for Accelerating Computational Protein Design" (with Y. Zhou, W. Xu, and M. Zeng). *Proc. International Conference on Intelligent Systems for Molecular Biology (ISMB)*, Boston, MA (July, 2014).

148. "Visualizing the Inter-domain Motions of a Flexible Protein Using Continuous Models" (with Y. Qi, J. Martin, and T. Oas). *Protein Science* 2014;**(23)**:113–114.

149. "Computing Conformational Entropy in Antibody Interfaces" (with P. Gainza, K. Roberts, and M. Hallen) *Biophysical Journal* 2014;106**(2)**:438a.

150. "Simultaneous determination of subunit and complex structures of symmetric homoöligomers from ambiguous NMR data" (with H. Chandola and C. Bailey-Kellogg). *Proceedings of the 4th ACM International Conference on Bioinformatics, Computational Biology, and Biomedical Informatics (ACM BCB)*. Washington, DC. September, 2013. ACM Press. pp. 171–180.

151. "Extracting Structural Information from Residual Chemical Shift Anisotropy: Analytic Solutions for Peptide Plane Orientations and Applications to Determine Protein Structure" (with C. Tripathy, A. Yan, and P. Zhou). *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Beijing, China (2013). In: *Research in Computational Molecular Biology*, Lecture Notes in Computer Science (LNBI), Springer-Verlag (Berlin), Volume 7821 (2013). pp. 271-284. $\frac{32}{161}$ acceptance rate.

152. "Design of Epitope-Specific Probes for Sera Analysis and Antibody Isolation" (with I. Georgiev, P. Acharya, S. Schmidt, Y. Li, D. Wycuff, G. Ofek, N. Doria-Rose, T. Luongo, Y, Yang, T. Zhou, J. Mascola, P. Kwong). B Cell Immunology and Antibody Functions, *AIDS Vaccine*. Boston, MA. Sep. 9-12 (2012).

153. "Design of Protein-protein Interactions with a Novel Ensemble-based Scoring Algorithm" (with K. Roberts, P. Cushing, P. Boisguerin, and D. Madden). In *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Vancouver, CA 2011. In *Lecture Notes in Computer Science*, Springer (Berlin), Volume 6577, pp. 361–376 (2011), DOI: 10.1007/978-3-642-20036-6. $\frac{43}{153}$ acceptance rate.

154. "A Geometric Arrangement Algorithm for Structure Determination of Symmetric Protein Homoöligomers from NOEs and RDCs" (with J. Martin, A. Yan, C. Bailey-Kellogg, and P. Zhou). In *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Vancouver, CA (2011). In *Lecture Notes in Computer Science*, Springer (Berlin), Volume 6577, pp. 222–237 (2011), DOI: 10.1007/978-3-642-20036-6 . $\frac{43}{153}$ acceptance rate.

155. "Protein Loop Closure using Orientational Restraints from NMR Data" (with C. Tripathy, J. Zeng, and P. Zhou). In *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Vancouver, CA (2011). In *Lecture Notes in Computer Science*, Springer (Berlin), Volume 6577, pp. 483–498 (2011), DOI: 10.1007/978-3-642-20036-6 . $\frac{43}{153}$ acceptance rate.

156. "A Bayesian Approach for Determining Protein Side-chain Rotamer Conformations using Unassigned NOE Data" (with J. Zeng, K. Roberts, and P. Zhou). In *Proceedings of the Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Vancouver, CA (2011). In *Lecture Notes in Computer Science*, Springer (Berlin), Volume 6577, pp. 563–578 (2011), DOI: 10.1007/978-3-642-20036-6 . $\frac{43}{153}$ acceptance rate.

157. "Algorithms and Analytic Solutions using Sparse Residual Dipolar Couplings for High-Resolution Automated Protein Backbone Structure Determination by NMR," (with A. Yershova, C. Tripathy, and P. Zhou), Workshop on the Algorithmic Foundations of Robotics (WAFR), Singapore (2010). $\frac{25}{60}$ acceptance rate.

158. "A Markov Random Field Framework for Protein Side-Chain Resonance Assignment" (with J. Zeng and P. Zhou). International Conference on Research in Computational Molecular Biology (RECOMB) 2010 (Lisbon). In *Lecture Notes in Computer Science*, Springer (Berlin) Volume LNBI 6044/2010, pp. 550–570. ISBN 978-3-642-12682-6. Acceptance rate less than $\frac{36}{175}$.

159. "NVR-BIP: Nuclear Vector Replacement using Binary Integer Programming for NMR Structure-Based Assignments" (with S. Apaydin, B. Catay, and N. Patrick). IEEE 24th International Symposium on Computer and Information Science (ISCIS). Cyprus, 14–16 September 2009.

160. "Algorithm for Backrub Motions in Protein Design" (with I. Georgiev, D. Keedy, J. Richardson, and D. Richardson). *Proc. International Conference on Intelligent Systems for Molecular Biology (ISMB)*, Toronto CA (July, 2008). 15% acceptance rate (out of ≥300).

161. "A Hausdorff-Based NOE Assignment Algorithm Using Protein Backbone Determined from Residual Dipolar Couplings and Rotamer Patterns," (with J. Zeng, C. Tripathy, and P. Zhou). *The Computational Systems Bioinformatics Conference (CSB),* Stanford CA. (August, 2008) pp. 169–181. $\frac{30}{135}$ acceptance rate.

162. "Dead-End Elimination with Backbone Flexibility" (with I. Georgiev), *Proc. International Conference on Intelligent Systems for Molecular Biology (ISMB)*, Vienna, Austria: July 21-25, 2007. 15% acceptance rate (out of 418).

163. "A Data-Driven, Systematic Search Algorithm for Structure Determination of Denatured or Disordered Proteins" (with L. Wang). *The Computational Systems Bioinformatics Conference (CSB),* Stanford CA. (August, 2006) pp. 67–78. $\frac{30}{156}$ acceptance rate.

     Winner of Best Paper Award.

164. "Improved Pruning Algorithms and Divide-and-Conquer Strategies for Dead-End Elimination, with Application to Protein Design" (with I. Georgiev and R. Lilien), *Proc. International Conference on Intelligent Systems for Molecular Biology (ISMB)*, Fortaleza, Brazil (August, 2006).

165. "Structure Determination of Symmetric Protein Complexes by a Complete Search of Symmetry Configuration Space Using NMR Distance Restraints" (with S. Potluri, A. Yan, J. Chou, and C. Bailey-Kellogg), Workshop on the Algorithmic Foundations of Robotics (WAFR), New York, NY. July 16-18, (2006). Pages 67-78. ISBN 1-86094-700-X.

166. "A Novel Minimized Dead-End Elimination Criterion and Its Application to Protein Redesign in a Hybrid Scoring and Search Algorithm for Computing Partition Functions over Molecular Ensembles," (with I. Georgiev and R. Lilien). *Proceedings of the Tenth Annual International Conference on Research in Computational Molecular Biology (RECOMB),* Venice, Italy (April 2–5, 2006). In Springer Berlin, Lecture Notes in Computer Science, RECOMB 2006, LNBI 3909, pp. 530–545, 2006. $\frac{40}{212}$ acceptance rate.

167. "An Efficient and Accurate Algorithm for Assigning Nuclear Overhauser Effect Restraints Using a Rotamer Library Ensemble and Residual Dipolar Couplings," (with L. Wang). The *IEEE Computational Systems Bioinformatics Conference (CSB)*, Stanford CA. (August, 2005) pp. 189–202. $\frac{30}{264}$ acceptance rate.

168. "An Algebraic Geometry Approach to Protein Backbone Structure Determination from NMR Data," (with L. Wang, and R. Mettu). The *IEEE Computational Systems Bioinformatics Conference (CSB)*, Stanford CA. (August, 2005) pp. 235–246. $\frac{38}{264}$ acceptance rate.

169. "High-Throughput Inference of Protein-Protein Interfaces from Unassigned NMR Data" (with R. Mettu and R. Lilien), *Proc. International Conference on Intelligent Systems for Molecular Biology (ISMB)*, Detroit, MI (2005) $\frac{56}{428}$ acceptance rate.

170. "Computational and physical modeling challenges in structural molecular biology and proteomics," *ACM Symposium on Solid and Physical Modeling* 2005: 7. Invited.

171. "Algorithmic Challenges in Structural Molecular Biology and Proteomics," Proc. Sixth International Workshop on the Algorithmic Foundations of Robotics (WAFR), Utrecht/Zeist, The Netherlands. July 11-13, 2004 pp. 1–10 (Invited).

172. "High-Throughput 3D Structural Homology Detection via NMR Resonance Assignment" (with C. Langmead), the *IEEE Computational Systems Bioinformatics Conference (CSB)*, Stanford CA, pp. 278–289 (August, 2004). $\frac{41}{202}$ acceptance rate.

173. "Analysis of a Systematic Search-Based Algorithm for Determining Protein Backbone Structure from a Minimal Number of Residual Dipolar Couplings" (with L. Wang), the *IEEE Computational Systems Bioinformatics Conference (CSB)*, Stanford CA, pp. 319–330 (August, 2004). $\frac{41}{202}$ acceptance rate.

174. "A Novel Ensemble-Based Scoring and Search Algorithm for Protein Redesign, and its Application to Modify the Substrate Specificity of the Gramicidin Synthetase A Phenylalanine Adenylation Enzyme," (with R. Lilien, B. Stevens, and A. Anderson), *Proceedings of the Eighth Annual International Conference on Research in Computational Molecular Biology (RECOMB),* San Diego (March 27-31, 2004) pp. 46-57. $\frac{38}{215}$ acceptance rate.

175. "3D Structural Homology Detection via Unassigned Residual Dipolar Couplings," (with C. Langmead), *Proc. IEEE Computational Systems Bioinformatics Conference (CSB)*, Stanford CA. (August 10, 2003) pp. 209-217. ISBN 0-7695-2000-6. $\frac{36}{151}$ acceptance rate.

176. "A Polynomial-Time Nuclear Vector Replacement Algorithm for Automated NMR Resonance Assignments," (with C. Langmead, A. Yan, R. Lilien, and L. Wang), *Proceedings of the Seventh Annual International Conference on Research in Computational Molecular Biology (RECOMB),* Berlin (2003) pp. 176–187. $\frac{35}{175}$ acceptance rate.

177. "Extracting Structural Information Using Time-Frequency Analysis of Protein NMR Data" (with C. Langmead), The Fifth Annual International Conference on Research in Computational Molecular Biology (RECOMB), Montreal, April 22–25 (2001) pp. 164–175. $\frac{35}{128}$ acceptance rate.

178. "Reducing Mass Degeneracy in SAR by MS (Structure-Activity Relation by Mass Spectrometry) by Stable Isotopic Labeling" (with C. Bailey-Kellogg, J. Kelley, and C. Stein) *Proc. 8th International Conference on Intelligent Systems for Molecular Biology (ISMB'2000)*, AAAI Press, (August 20–23, 2000) La Jolla, CA, pp. 13–24. $\frac{40}{140}$ acceptance rate.

179. "The NOESY Jigsaw: Automated Protein Secondary Structure and Main-Chain Assignment from Sparse, Unassigned NMR Data," (with C. Bailey-Kellogg, A. Widge, J. Kelley, M. Berardi, and J. Bushweller), The Fourth Annual International Conference on Research in Computational Molecular Biology (RECOMB), Tokyo, Japan, April 8 — 11, 2000, pp. 33–44. 33% acceptance rate.

180. "Physical Geometric Algorithms for Structural Molecular Biology" (with C. Bailey-Kellogg, J. Kelley, and R. Lilien) invited paper at the Special Session on Computational Biology & Chemistry, Proc. IEEE International Conference on Robotics and Automation (ICRA)(2001), Seoul, Korea, pp. 940-947.

B. Systems Biology

181. "A Maximum Entropy Algorithm for Rhythmic Analysis of Genome-Wide Expression Patterns", (with C. Langmead and C. R. McClung), Proc. IEEE Computer Society Bioinformatics Conference (CSB), Stanford University, Palo Alto, (August 14–16, 2002) pp. 237–245. Acceptance rate: $\frac{19}{103}$.

182. "Phase-Independent Rhythmic Analysis of Genome-Wide Expression Patterns", (with C. Langmead, A. Yan, and C. R. McClung), Proceedings of The Sixth Annual International Conference on Research in Computational Molecular Biology (RECOMB), Washington DC (2002). pp. 205–215. Acceptance rate: $\frac{35}{118}$.

Note: Some papers in § 14.6.1A *also relate to Systems Biology.*

14.6.2   Neuroscience

183. "Efficient coding of vocal transitions revealed by sparse synaptic activity in the singing bird" (with K. Hamaguchi, I. Yoon, and R. Mooney). *Neuroscience*, Society for Neuroscience Conference. New Orleans, Oct. 13-17, 2012.

14.6.3   Microelectromechanical Systems (MEMS)

184. "Turning-rate Selective Control: A New Method for Independent Control of Stress-engineered MEMS Microrobots" (with C. Levey and I. Paprotny). Proceedings of *Robotics: Science and Systems Conference (RSS)*, University of Sydney, Sydney, NSW, Australia. July 9-13, 2012. $\frac{61}{185}$ acceptance rate.

185. "Simultaneous Control of Multiple MEMS Microrobots" (with C. Levey, I. Paprotny, and D. Rus). Proceedings of the Eighth International Workshop on the Algorithmic Foundations of Robotics (WAFR), Guanajuato, México, December 7–9, 2008.

186. "Assembly of Planar Structures by Parallel Actuation of MEMS Microrobots (with C. Levey and I. Paprotny). *Hilton Head Workshop: A Solid-State Sensors, Actuators and Microsystems Workshop* 2008, pp. 202–207; Hilton Head, SC.

187. "A Steerable, Untethered, 250×60 μm MEMS Mobile Micro-Robot," (with C. Levey, C. McGray, I. Paprotny, and D. Rus). 12th *International Symposium of Robotics Research (ISRR),* October 12-15, 2005, San Francisco, CA.

188. "Untethered Micro-Actuators for Autonomous Micro-robot Locomotion: Design, Fabrication, Control, and Performance" (with C. Levey, C. McGray, D. Rus, and M. Sinclair). 11th *International Symposium of Robotics Research (ISRR),* October 19-22, 2003, Siena, Italy.

189. "Power Delivery and Locomotion of Untethered Micro-Actuators," (with C. Levey, C. McGray, D. Rus, and M. Sinclair) *IEEE MEMS (Proc. IEEE International Conference on Micro Electro Mechanical Systems)*, Kyoto, Japan (January 19-23, 2003) pp. 124-129.

190. "Fully Programmable MEMS Ciliary Actuator Arrays for Micromanipulation Tasks," (with J. Suh, R. B. Darling, K.-F. Böhringer, H. Baltes, and G. Kovacs), Proceedings of the IEEE International Conference on Robotics and Automation (ICRA), San Francisco (April, 2000) pp. 1101–1108.

191. "A Single Universal Force Field can Uniquely Pose any Part up to Symmetry," (with K.-F. Böhringer, F. Lamiraux, and L. Kavraki), 9th *International Symposium of Robotics Research (ISRR)*, Snowbird, Utah, October 9-12 (1999).

192. *Algorithmic MEMS*, (with K.-F. Böhringer), 3rd *International Workshop on the Algorithmic Foundations of Robotics (WAFR),* Houston, TX (March, 1998).

193. "Vector Fields for Task-Level Distributed Manipulation: Experiments with Organic Micro Actuator Arrays," (with K.-F. Böhringer, J. Suh, and G. Kovacs) in *Proc. IEEE International Conference on Robotics and Automation,* Albuquerque, NM, (1997) pp. 1779–1786.

194. "Upper and lower bounds for programmable vector fields with applications to MEMS and vibratory plate parts feeders," (with K.-F. Böhringer and N. MacDonald), Proc. *International Workshop on the Algorithmic Foundations of Robotics (WAFR),* Toulouse, France, July 1996.

195. "Classification and Lower Bounds for MEMS Arrays and Vibratory Parts Feeders: What Programmable Vector Fields Can (and Cannot) Do," *IEEE International Conference on Robotics and Automation (ICRA),* Minneapolis, Minnesota (April 1996) (with K.-F. Böhringer and N. C. MacDonald).

196. "Single-Crystal Silicon Actuator Arrays for Micro-Manipulation Tasks," (with K.-F. Böhringer and N. C. MacDonald),*IEEE Workshop on Micro Electro Mechanical Systems (MEMS),* San Diego, California (February, 1996).

197. "Sensorless Manipulation Using Massively Parallel Micro-fabricated Actuator Arrays," (with K.-F. Böhringer, R. Mihailovich, and Noel C. MacDonald), *Proc. IEEE International Conference on Robotics and Automation*, San Diego, CA (May, 1994).

198. "A Theory of Manipulation and Control for Microfabricated Actuator Arrays," (with K.-F. Böhringer, R. Mihailovich, and Noel C. MacDonald) in Proc. 7th IEEE Workshop on Micro Electro Mechanical Systems (MEMS'94). Kanagawa, Japan (January, 1994).

14.6.4 Computer Graphics and Haptics

199. "Accessible Animation and Customizable Graphics via Simplicial Configuration Modeling" (with T. Ngo, D. Cutrell, J. Dana, L. Loeb, and S. Zhu), in Proc. ACM SIGGRAPH – the 27th International Conference on Computer Graphics and Interactive Techniques (New Orleans) July, 2000, pp. 403–410.

200. "Using Haptic Vector Fields for Animation Motion Control," (with F. Henle), Proceedings of the IEEE International Conference on Robotics and Automation (ICRA), San Francisco (April, 2000) pp. 3435–3442.

201. "Real-Time Robot Motion Planning Using Rasterizing Computer Graphics Hardware", (with J. Lengyel, M. Reichert, and D. Greenberg), *Proc. ACM SIGGRAPH '90*, Dallas, TX (Aug 1990), pp. 327-336.

202. *BUILDER: A Database and Display Program for Computer-aided Architectural Design. (A system for representation and display of design problems in architecture and urban design).* Harvard Computer Graphics Conference, (Session 17, Architectural Practice) July 27, 1982. Cambridge, MA. (Oral conference presentation; no associated paper, but see Technical Report, Publication # 291 below). Scanned 35 mm slides: `www.cs.duke.edu/brd/Historical/hlcg/`

14.6.5 Robotics and Motion Planning

203. "Distributed Manipulation of Multiple Objects Using Ropes," (with L. Gariepy and D. Rus), Proceedings of the IEEE International Conference on Robotics and Automation (ICRA), San Francisco (April,

2000) pp. 450–457.

204. "Practical Mobile Robot Self-Localization," (with J. Howell), Proceedings of the IEEE International Conference on Robotics and Automation (ICRA), San Francisco (April, 2000) pp. 3485–3492.

205. "Experiments in Constrained Prehensile Manipulation: Distributed Manipulation with Ropes," (with L. Gariepy and D. Rus) *International Symposium on Experimental Robotics (ISER)*, Sydney, Australia (1999).

206. "Robust geometric algorithms for sensor planning," (with A. Briggs), *International Workshop on the Algorithmic Foundations of Robotics (WAFR),* Toulouse, France, July 1996.

207. "Moving Furniture with Teams of Automonous Mobile Robots," (with J. Jennings and D. Rus), *Proc. IEEE/Robotics Society of Japan International Workshop on Intelligent Robots and Systems*, Pittsburgh, PA (1995). pp. 235–242.

208. "Distributed Robotic Manipulation: Experiments in Minimalism," *International Symposium on Experimental Robotics*, Stanford, CA (1995).

209. "Information Invariants for Distributed Manipulation" (with J. Jennings and D. Rus) in *The First Workshop on the Algorithmic Foundations of Robotics (WAFR)*, San Francisco, CA (1994).

210. "Automatic Sensor Configuration for Task-Directed Planning," (with A. J. Briggs), *Proc. IEEE International Conference on Robotics and Automation*, San Diego, CA (May, 1994).

211. "Analyzing Teams of Cooperating Mobile Robots," (with J. Jennings and D. Rus), *Proc. IEEE International Conference on Robotics and Automation*, San Diego, CA (May, 1994).

212. "Towards a Theory of Information Invariants for Cooperating Autonomous Mobile Robots," (with J. Jennings and D. Rus) International Symposium of Robotics Research (ISRR). Hidden Valley, PA (October 2, 1993).

213. "Mobile Robots, Map-making, Shape Metrics, and Localization," (with R. Brown and P. Chew). International Association of Science and Technology for Development (IASTED) International Conference on Robotics and Manufacturing, (Oxford, England) (September 23-25, 1993).

214. "Experimental Information Invariants for Cooperating Autonomous Mobile Robots," (with J. Jennings and D. Rus) International Joint Conference on Artificial Intelligence (IJCAI) Workshop on Dynamically Interacting Robots. Chambery, France (Aug 28, 1993).

215. "Information Invariants in Robotics: Part I – State, Communication, and Side-Effects," *Proc. IEEE International Conference on Robotics and Automation*, Atlanta, May (1993).

216. "Information Invariants in Robotics: Part II – Sensors and Computation," *Proc. IEEE International Conference on Robotics and Automation*, Atlanta, May (1993).

217. "Constructive Recognizability for Task-Directed Robot Programming", (with J. Jennings), *Proc. IEEE International Conference on Robotics and Automation*, Nice, France (May, 1992), pp. 2446-2452.

218. "Program Mobile Robots in Scheme," (with J. Rees) *Proc. IEEE International Conference on Robotics and Automation*, Nice, France (May, 1992), pp. 2681-2688.

219. "Programming Autonomous Agents: A Theory of Perceptual Equivalence" (with J. Jennings), 1$^{\text{st}}$ AAAI Fall Symposium on Sensory Aspects of Robotic Intelligence, Asilomar, CA (Nov, 1991). (Invited)

220. "Perceptual Limits, Perceptual Equivalence Classes, and a Robot's Sensori-Computational Capabilities", (with J. Jennings), *IEEE/Robotics Society of Japan International Workshop on Intelligent Robots and Systems*, Osaka, Japan (Nov. 1991), pp. 1397-1405.

221. "Sensor Interpretation and Task-Directed Planning Using Perceptual Equivalence Classes," (with J. Jennings) *Proc. IEEE International Conference on Robotics and Automation*, Sacramento, CA (April, 1991), pp. 190–197.

222. "Time-Safety Trade-offs and a Bang-Bang Algorithm for Kinodynamic Planning," (with P. Xavier) *Proc. IEEE International Conference on Robotics and Automation*, Sacramento, CA (April, 1991), pp. 552-557.

223. "On The Motion of Compliantly-Connected Rigid Bodies in Contact: A System for Analyzing Designs for Assembly", (with D. Pai), *Proc. IEEE International Conference on Robotics and Automation*, Cincinatti, Ohio (May 1990) pp. 1756–1763.

224. "Near-Optimal Kinodynamic Planning for Robots With Coupled Dynamics Bounds", (with P. Xavier), *Fourth IEEE International Symposium on Intelligent Control*, (Sept. 24-26, 1989) Albany, NY (Invited). pp. 354-359.

225. "A Provably Good Approximation Algorithm for Optimal-Time Trajectory Planning" , (with P. Xavier) *Proc. IEEE International Conference on Robotics and Automation*, Scottsdale, Arizona. (May 1989). pp. 958–964.

226. "Towards Experimental Verification of an Automated Compliant Motion Planner based on a Geometric Theory of Error Detection and Recovery", (with J. Jennings, D. Campbell) *Proc. IEEE International Conference on Robotics and Automation*, Scottsdale, Arizona. (May 1989). pp. 632–637.

227. "Planning Multi-Step Error Detection and Recovery Strategies", *Proc. IEEE International Conference on Robotics and Automation*, Philadelphia, PA April, 1988, pp. 892-897.

228. "A Theory of Error Detection and Recovery: Robot Motion Planning with Uncertainty in the Geometric Models of the Robot and Environment", *International Workshop on Geometric Reasoning, Oxford University, England.* June, 1986 (Invited).

229. "Robot Motion Planning with Uncertainty in the Geometric Models of the Robot and Environment: A Formal Framework for Error Detection and Recovery", *Proc. IEEE International Conference on Robotics and Automation*, San Francisco, CA April, 1986 (Invited).

230. "On Motion Planning with Six Degrees of Freedom: Solving the Intersection Problems in Configuration Space", *Proc. IEEE International Conference on Robotics and Automation*, St. Louis, Missouri (1985).

231. "The Mover's Problem in Automated Structural Design", *Proc. Harvard Computer Graphics Conference*, Cambridge, MA 1983, (Invited).

14.6.6   Computational Geometry

232. "Some Geometric and Computational Challenges Arising in Structural Molecular Biology (Invited Talk)." 35th International Symposium on Computational Geometry (SoCG 2019). Leibniz International Proceedings in Informatics (LIPIcs), vol. 129. pp. 2:1–2:1. Schloss Dagstuhl–Leibniz-Zentrum für Informatik. doi: 10.4230/LIPIcs.SoCG.2019.2

233. *On the Area Bisectors of a Polygon*, (with K.-F. Böhringer and D. Halperin) Second CGC Workshop on Computational Geometry, (October 18-19, 1997) Duke University, Durham, NC.

234. "The Area Bisectors of a Polygon and Force Equilibria in Programmable Vector Fields," (with K.-F. Böhringer and D. Halperin) *Proc.* 13th *ACM Symposium on Computational Geometry,* Nice, France (1997) pp. 457–459.

235. "A Rational Rotation Method for Robust Geometric Algorithms", (with J. Canny and G. Ressler), *Proc. ACM Symposium on Computational Geometry*, Berlin, BRD (June, 1992), pp. 251-260.

236. "On the Complexity of Computing the Homology Type of a Triangulation", (with D. Chang), *IEEE Symposium on the Foundations of Computer Science*, San Juan, (October 1991), pp. 650-661.

237. "Provably Good Approximation Algorithms for Optimal Kinodynamic Planning for Cartesian Robots and Open Chain Manipulators", (with P. Xavier), *Proc.* 6th *ACM Symposium on Computational Geometry*, Berkeley, CA (June 6, 1990), pp. 290-300.

238. "On The Complexity of Kinodynamic Planning", (with J. Canny, J. Reif, and P. Xavier) 29th *Symposium on the Foundations of Computer Science*, White Plains, NY (1988). pp. 306-316.

239. "The Complexity of Planar Compliant Motion Planning with Uncertainty", *Proc.* 4th *ACM Symposium on Computational Geometry*, Urbana, IL June, 1988, pp. 309-318.

240. "Simplified Voronoi Diagrams", (with John Canny) *Proc. Third ACM Symposium on Computational Geometry*, Waterloo, Ontario (June 1987), pp. 153-161.

14.7   Articles and Chapters in Multiply-Authored Books

241. "MicroStressBots: Species Differentiation in Surface Micromachined Microrobots" (with I. Paprotny and C. Levey). In *Small-Scale Robotics. From Nano-to-Millimeter-Sized Robotic Systems and Applications*, LNAI 8336, Lecture Notes in Computer Science, Volume 8336, Springer-Verlag (2014), pp. 66–80.

242. "The Compass That Steered Robotics." In *Logic and Program Semantics*, Lecture Notes in Computer Science (LNCS) 7230, Springer-Verlag (Berlin) 2012. pp. 50–65.

243. "Algorithms and Analytic Solutions using Sparse Residual Dipolar Couplings for High-Resolution Automated Protein Backbone Structure Determination by NMR," (with A. Yershova, C. Tripathy, and P. Zhou). In *Algorithmic Foundations of Robotics, IX*, Springer Tracts in Advanced Robotics, Vol. 68

(2011) pp. 255–372.

244. "Simultaneous Control of Multiple MEMS Microrobots" (with C. Levey, I. Paprotny, and D. Rus). In *Springer Tracts on Advanced Robotics,* **57**, Springer-Verlag (Berlin), (2010), pp. 69–84.

245. "Structure Determination of Symmetric Protein Complexes by a Complete Search of Symmetry Configuration Space Using NMR Distance Restraints" (with S. Potluri, A. Yan, J. Chou, and C. Bailey-Kellogg). In *Algorithmic Foundation of Robotics VII*. Springer Tracts in Advanced Robotics (vol. 47), Ed. S. Akella *et al.* Springer-Verlag (Berlin) 2008 pp. 335–340.

246. "A Steerable, Untethered, 250×60 μm MEMS Mobile Micro-Robot" (with C. Levey, C. McGray, I. Paprotny and D. Rus). In *Robotics Research: Results of the* 12th *International Symposium ISRR*, Springer Tracks in Advanced Robotics 28, Ed. S. Thrun *et al..* Springer-Verlag (Berlin) 2007 pp. 337–356.

247. "Algorithmic Challenges in Structural Molecular Biology and Proteomics," in *Algorithmic Foundations of Robotics VI*, Springer Tracts in Advanced Robotics (vol. 17), eds. M. Erdmann *et al.*, Springer (Berlin) 2005, pp. 1–10.

248. "Untethered Micro-Actuators for Autonomous Micro-robot Locomotion: Design, Fabrication, Control, and Performance" (with C. Levey, C. McGray, D. Rus, and M. Sinclair). in *Robotics Research*, eds. P. Dario and R. Chatila. Springer-Verlag (London) 2005, pp. 502–516.

249. "Distributed Manipulation of Multiple Objects Using Ropes" (with L. Gariepy and D. Rus). In *Multi-Robot Systems: From Swarms to Intelligent Automata*, Ed. A. Schultz and L. Parker. Kluwer Academic Publishing (Netherlands) 2002, pp. 83–90.

250. "A Single Universal Force Field Can Uniquely Orient Non-symmetric Parts," (with K.-F. Böhringer, F. Lamiraux, and L. Kavraki), in *Robotics Research*, eds. J. Hollerbach and D. Koditschek, Springer-Verlag (London) 2000, pp. 395–402.

251. "CMOS Integrated Organic Ciliary Actuator Arrays for General-Purpose Micromanipulation Tasks," (with J. Suh, R. B. Darling, K.-F. Böhringer, H. Baltes, and G. Kovacs), in *Distributed Manipulation*, ed. K. Böhringer et al., Kluwer Academic Publishing (2000), pp. 191–216.

252. "A Distributed, Universal Device for Planar Parts Feeding: Unique Part Orientation in Programmable Force Fields," (with K.-F. Böhringer, F. Lamiraux, and L. Kavraki), in *Distributed Manipulation*, ed. K. Böhringer et al., Kluwer Academic Publishing (2000), pp. 1–28.

253. "Constrained Prehensile Manipulation: Distributed Manipulation with Ropes" (with L. Gariepy and D. Rus), in *Distributed Manipulation*, ed. K. Böhringer et al., Kluwer Academic Publishing (2000), pp. 29–48.

254. "Experiments in Constrained Prehensile Manipulation: Distributed Manipulation with Ropes" (with L. Gariepy and D. Rus), in *Experimental Robotics VI*, Lecture Notes in Control and Information Sciences, vol. 250, ed. P. Corke et al., Springer-Verlag, 2000, pp. 25–36.

255. "Algorithmic MEMS," (with K.-F. Böhringer) in *Robotics: The Algorithmic Perspective*, ed. P. Agarwal, L. Kavraki, and M. Mason, A. K. Peters, Natick, MA (1998). pp. 1–20.

256. "Upper and lower bounds for programmable vector fields with applications to MEMS and vibratory plate parts feeders," (with K.-F. Böhringer and N. MacDonald), in *Algorithms for Robotic Motion and Manipulation,*, ed. J. P. Laumond and M. Overmars, A. K. Peters, Wellesley, MA (1997). pp. 255–276.

257. "Robust geometric algorithms for sensor planning," (with A. Briggs), in *Algorithms for Robotic Motion and Manipulation,*, ed. J. P. Laumond and M. Overmars, A. K. Peters, Wellesley, MA (1997). pp. 197–212.

258. "Distributed Robotic Manipulation: Experiments in Minimalism" (with K. F. Böhringer, R. Brown, J. Jennings, and D. Rus), in *Experimental Robotics IV*, Lecture Notes in Control and Information Sciences 223, ed. O. Khatib *et al.*, Springer Verlag (Berlin) 1997 pp. 11–25.

259. "On Information Invariants in Robotics," in *Computational Theories of Interaction and Agency,* MIT Press (1996), ed., P. Agre and S. Rosenschein.

260. "Information Invariants for Distributed Manipulation" (with J. Jennings and D. Rus) in *Algorithmic Foundations of Robotics*, A. K. Peters, Boston, MA ed. K. Goldberg *et al.* (1995). pp. 431–458.

261. "A Geometric Approach to Error Detection and Recovery for Robot Motion Planning with Uncertainty", in *Geometric Reasoning*, MIT Press, Cambridge (1989), pp. 223-274.

262. "Simplified Voronoi Diagrams", (with John Canny), in *Autonomous Robot Vehicles*, Springer-Verlag,

New York: (1990), pp. 272-289.

263. "Symbolic Methods for the Simulation of Planar Mechanical Systems in Design", (with D. Pai), in *Symbolic and Numerical Computation for Artificial Intelligence*, (ed. B. Donald *et al.*) Academic Press, Harcourt Jovanovich, (London: 1992), pp. 245-258.

14.8 Selected Invited Papers

264. "Spatial Aggregation in Scientific Data Mining," (with C. Bailey-Kellogg and F. Zhao), First SIAM Conference on Computational Science and Engineering, September 21-24, 2000, Wyndham City Center Hotel, Washington, DC.

265. "Haptics for Animation Motion Control" (with F. Henle), The Fourth PHANTOM Users Group Workshop (PUG99), October 9-12, 1999 (Massachusetts Institute of Technology). Received Best Paper Award.

266. "Prototyping Animation Motion Control with Haptic Programmable Force Fields", Workshop on "Motion Support in Virtual Prototyping," (with Fred Henle) Stanford, May 5-7, 1999.

267. "CMOS Integrated Organic Ciliary Array as a General-Purpose Micromanipulation Tool," (with J. Suh, R. B. Darling, K.-F. Böhringer, H. Baltes, and G. Kovacs), IEEE International Conference on Robotics and Automation, Workshop on Distributed Manipulation (Detroit) May 11, 1999.

268. "Part Orientation with One or Two Stable Equilibria Using Programmable Vector Fields," (with K.-F. Böhringer, F. Lamiraux, and L. Kavraki), IEEE International Conference on Robotics and Automation, Workshop on Distributed Manipulation (Detroit) May 11, 1999.

269. "Experiments in Constrained Prehensile Manipulation: Distributed Manipulation with Ropes," (with L. Gariepy and D. Rus) IEEE International Conference on Robotics and Automation, Workshop on Distributed Manipulation (Detroit) May 11, 1999.

270. "Micro Contacts and Micro Manipulation with MEMS Actuator Arrays" (with K.-F. Böhringer) IEEE International Conference on Robotics and Automation, Workshop on Modeling, Contact Analysis, and Simulation of Mechanical Systems in Robotics and Manufacturing, (Belgium, 1998).

14.9 Conference Abstracts that were Selected for Oral Presentation

Note: In the life sciences, conference abstracts are submitted, and only a few are chosen for oral presentation. This choice is made by a program committee of 5-8 senior scientists, and is a form of recognition in the field. Oral presentations are highly selective, especially in the premier conferences such as 3DSIG/ISMB, typically less than 10-15% of submissions. There is usually a conference proceedings published of 1-2 pages per abstract.

"OSPREY 3.0: Open-Source Protein Redesign for You, with Powerful New Features" (with J. Martin, A. Lowegard, M. Frenkel, M.. Hallen, A. Ojewole, J. Jou, S. Wang, and G. Holt). Structural Bioinformatics and Computational Biophysics (3DSIG) track of ISMB. Chicago, Il. July 6-12, 2018. (Selected for Oral Presentation).

"Improving Minimized Protein Design Efficiency with Partitioned Continuous Rotamers" (with K. Roberts). Structural Bioinformatics and Computational Biophysics (3DSIG), ISMB Satellite Meeting, Boston, MA July 11-12, 2014. (Selected for Oral Presentation).

Winner of Best Poster Award.

"Design of Peptide Inhibitors of CFTR-associated Protein CAL" (with K. Roberts, P. Cushing, and D. Madden). Structural Bioinformatics and Computational Biophysics (3DSIG), ISMB Satellite Meeting, Boston, MA July 2010. (Selected for Oral Presentation).

"Algorithms for Protein Design" (with I. Georgiev and C. Chen). Structural Bioinformatics and Computational Biophysics (3DSIG), ISMB Satellite Meeting, Stockholm, Jun 27-28 2009. (Selected for Oral Presentation).

"High-throughput structure determination using sparse NMR data" (with L. Wang). 5th NIH/NIGMS Protein Structure Initiative "Bottlenecks" Workshop, Natcher Conference Center, NIH, Bethesda, Maryland. April 13-14, 2006. Selected for oral presentation.

14.10 Selected Conference Abstracts and Posters

We have so many posters that I have stopped keeping track of them. Here are a few from before 2013:

"Solution structure of trimeric HIV-1 gp41 MPER using hybrid computational methods." J. Martin, P. Reardon, L. Spicer, and B. R. Donald. Gordon Research Conference: Computational Aspects of Biomolecular NMR. Mount Snow, VT, 2013.

"Computational Protein Design of Improved HIV Antibodies." K.E. Roberts and B.R. Donald. Duke Computational Biology and Bioinformatics Program Retreat. October 6, 2012.

"NMR Structure Determination of GrsA Epimerase Domain by Residual Dipolar Couplings (RDCs), Sparse NOEs and PREs." C.-Y. Chen, C. Tripathy, J. Zeng, P. Zhou and B. R. Donald. 2012 Annual Biochemistry Retreat, Wrightsville Beach, North Carolina. October 5-7, 2012.

"Towards Entirely RDC-Based Protein Backbone Structure Determination." J. W. Martin and B. R. Donald. Biochemistry Department Retreat, Wrightsville Beach, North Carolina. October 5-7, 2012.

"Protein design with more realistic continuous flexibility." M. A. Hallen, D. A. Keedy and B. R. Donald. Duke University Medical Center Biochemistry Department Retreat, Wrightsville Beach, North Carolina. October 5-7, 2012.

"Computational Protein Design of Improved HIV Antibodies." K.E. Roberts and B.R. Donald. Duke Biochemistry Department Retreat. October 5-6, 2012.

"Towards Entirely RDC-Based Protein Backbone Structure Determination." J. W. Martin and B. R. Donald. Computer Science Department Retreat, Beaufort, North Carolina. September 21-23, 2012.

"Predicting drug-resistance on a computer using OSPREY" P. Gainza, K.M. Frey, I. Georgiev, A.C. Anderson, B.R. Donald. Duke Computer Science Retreat, Beaufort, NC, September 2012.

"Rare NADPH epimer that may be linked to MRSA drug resistance discovered through computational protein design" P. Gainza, K.M. Frey, I. Georgiev, A.C. Anderson, B.R. Donald. Duke Biochemistry Retreat, Wrightsville, NC, September 2012.

"Packing Protein Secondary Structure Elements Without Distance Restraints." J. W. Martin and B. R. Donald. Computer Science Department Poster Session, Durham, North Carolina. February 17, 2012.

"Improved modeling in protein design algorithms and its application to predict drug-resistance mutations" P. Gainza, K.E. Roberts, K.M. Frey, I. Georgiev, A.C. Anderson, B.R. Donald. Duke Computer Science Recruitment, Durham, NC, February 2012.

"NMR Structure Determination of GrsA Epimerase Domain by Residual Dipolar Couplings (RDCs) and Sparse NOE Data." C.-Y. Chen, C. Tripathy, J. Zeng, A. Yershova, P. Zhou and B. R. Donald. 2011 Annual Biochemistry Retreat, Wrightsville Beach, North Carolina. November 11-13, 2011.

"Dead-End Elimination with Perturbations ('DEEPer'): A provable protein design algorithm with continuous sidechain and backbone flexibility." M. A. Hallen, D. A. Keedy and B. R. Donald. Duke University Medical Center Biochemistry Department Retreat, Wrightsville Beach, North Carolina. November 11-13, 2011.

"Packing Protein Secondary Structure Elements Without Distance Restraints." J. W. Martin and B. R. Donald. Biochemistry Department Retreat, Wrightsville Beach, North Carolina. November 11-13, 2011.

"NMR Structure Determination of GrsA Epimerase Domain by Residual Dipolar Couplings (RDCs) and Sparse NOE Data." C.-Y. Chen, C. Tripathy, J. Zeng, A. Yershova, P. Zhou and B. R. Donald. 2011 Duke Basic Science Day, Durham, North Carolina. October 10, 2011.

"Protein Design Using Continuous Rotamers." K.E. Roberts, P. Gainza and B.R. Donald. Duke Computational Biology and Bioinformatics Program Retreat. September 24, 2011.

"NMR structural inference of symmetric homo-oligomers" (with H. Chandola and C. Bailey-Kellogg).Structural Bioinformatics and Computational Biophysics (3DSIG), ISMB Satellite Meeting, Boston, MA July 2010.

"Applying 4-D Sparse Sampling and FFT-CLEAN Processing to NMR Studies of Large Proteins" (with B. Coggins, J. Werner-Allen, C.-Y. Chen, and P. Zhou). 51st Experimental Nuclear Mag-

netic Resonance Conference, Daytona Beach, Florida. April 18-23, 2010.

"RDC-PANDA: a High-Resolution NMR Structure Determination Algorithm Starting with a Global Fold Calculated from Exact Solutions to the RDC Equations" (with J. Zeng, J. Boyles, C. Tripathy, L. Wang, A. Yan, and P. Zhou). 51st Experimental Nuclear Magnetic Resonance Conference, Daytona Beach, Florida. April 18-23, 2010.

"A Markov Random Field Algorithm for Protein Side-Chain Resonance Assignment" (with J. Zeng, and P. Zhou). 51st Experimental Nuclear Magnetic Resonance Conference, Daytona Beach, Florida. April 18-23, 2010.

"RDC-PANDA: a High-Resolution NMR Structure Determination Algorithm Starting with a Global Fold Calculated from Exact Solutions to the RDC Equations" (with J. Zeng, J. Boyles, C. Tripathy, L. Wang, A. Yan, and P. Zhou). 14th Annual International Conference on Research in Computational Molecular Biology (RECOMB), Lisbon, Portugal. April 25-28, 2010.

"NVR-BIP: Nuclear Vector Replacement using Binary Integer Programming for NMR Structure-Based Assignments (with Mehmet Serkan Apaydin, Bulent Catay, and Nicholas Patrick). 14th Annual International Conference on Research in Computational Molecular Biology (RECOMB), Lisbon, Portugal. April 25-28, 2010.

"Computational and experimental scanning and redesign of nucleic acid binding proteins" (with F. Reza, Q. Wang, I. Georgiev, and J. Tian). Sigma Xi, The Scientific Research Society 2009 Annual Meeting and International Research Conference, The Woodlands in Houston, Texas. November 12-15, 2009.

"Molecular ensemble engineering and evaluation for targeted genome therapeutics" (with F. Reza, Q. Wang, I. Georgiev, and J. Tian). Biomedical Engineering Society 2009 Annual Meeting, Pittsburgh, Pennsylvania. October 7-10, 2009.

"DNA-protein molecular ensemble engineering and evaluation" (with F. Reza, Q. Wang, I. Georgiev, and J. Tian). Duke University Center for Biomolecular and Tissue Engineering Kewaunee Event, Durham, North Carolina. April 23, 2009.

"Modeling and engineering of nanomolecular interactions" (engineering structure-function interactions in collaboration with F. Reza, Q. Wang, I. Georgiev, and J. Tian). Sigma Xi, The Scientific Research Society 2008 Annual Meeting and Student Research Conference, Washington, District of Columbia. November 20-23, 2008.

"Algorithms for Protein Design" (with I. Georgiev and C. Chen). Duke University Department of Computer Science Retreat, Beaufort, NC, 19-21 Sep 2008.

"Visualizing RDC Solution Curves in their Structural Context" (with V. B. Chen, A. Yan, J. N. Block, D. .C. Richardson, and J .S. Richardson). NIH/NIGMS Protein Structure Initiative "Bottlenecks" Workshop, Natcher Conference Center, NIH, Bethesda, Maryland. April 14-16, 2008.

"High-Resolution Structure Determination Starting with a Global Fold Calculated from Exact Solutions to the RDC Equations" (with J. Zeng, J. Boyles, A. Yan, and P. Zhou). 2008 NIH/NIGMS Protein Structure Initiative "Bottlenecks" Workshop, Natcher Conference Center, NIH, Bethesda, Maryland. April 14-16, 2008.

"Robust Structure Based Protein NMR Assignments Using Native Ensembles" (with S. Apaydın and V. Conitzer). Biochemistry Department Retreat, Wrightsville Beach, NC, October 12-14, 2007.

"Bridging the Protein Gap: Using a Fragment Library with Incomplete NMR Models," (with V. Chen, C. Tripathy, P. Zhou, D. Richardson, and J.. Richardson). Biochemistry Department Retreat, Wrightsville Beach, NC, October 12-14, 2007.

"Algorithms for NOE Assignment and Structure Determination from RDCs," (with J. Zeng, C. Tripathy, and P. Zhou). Biochemistry Department Retreat, Wrightsville Beach, NC, October 12-14, 2007.

"NMR Structure Determination of Symmetric Homo-oligomers by a Complete Search Algorithm using NOEs, RDCs, and CSA," (with A. Yan, S. Potluri, and C. Bailey-Kellogg). Biochemistry Department Retreat, Wrightsville Beach, NC, October 12-14, 2007.

"Kinetic & Structural Studies of the Initiation Module, PheATE, of Wild Type & Redesigned Gramicidin S Synthetase," (with C-Y. Chen, J. MacMaster, and I. Georgiev). Biochemistry Department Retreat, Wrightsville Beach, NC, October 12-14, 2007.

"Computational Redesign of the Phenylalanine Adenylation Domain of Gramicidin S Synthetase," (with I. Georgiev, C-Y. Chen, and J. MacMaster). Biochemistry Department Retreat, Wrightsville Beach, NC, October 12-14, 2007.

"Robust Structure-based Assignments Using Native Ensembles" (with S. Apaydın). 6th NIH/NIGMS Protein Structure Initiative "Bottlenecks" Workshop, Natcher Conference Center, NIH, Bethesda, Maryland. March 19-20, 2007.

"Structure Determination of Symmetric Homo-Oligomers by a Complete Search of Symmetry Configuration Space Using NMR Restraints from NOEs and RDCs." (with A. Yan, S. Potluri, and C. Bailey-Kellogg). 6th NIH/NIGMS Protein Structure Initiative "Bottlenecks" Workshop, Natcher Conference Center, NIH, Bethesda, Maryland. March 19-20, 2007.

"Automated Structure Determination from Sparse NMR Data" (with J. Zeng, L. Wang, C. Tripathy, and P. Zhou). 6th NIH/NIGMS Protein Structure Initiative "Bottlenecks" Workshop, Natcher Conference Center, NIH, Bethesda, Maryland. March 19-20, 2007.

"Structure Determination of Symmetric Homo-oligomers Using NMR Restraints and van der Waals Packing" (with S. Potluri, A. Yan, J. Chou, and C. Bailey-Kellogg). First Annual IGSP Retreat, Grandover Resort, Greensboro, NC. November 3-4, 2006.

> Winner of Best Poster Award.

"Improved Pruning Algorithms for Dead-End Elimination, with Application to Protein Design" (with I. Georgiev and R. Lilien). First Annual IGSP Retreat, Grandover Resort, Greensboro, NC. November 3-4, 2006.

"Predicting Protein Folding Kinetics from the Denatured Ensemble of ACBP using Stochastic Roadmap Simulation" (with C. Tripathy, S. Apaydin and L. Wang). First Annual IGSP Retreat, Grandover Resort, Greensboro, NC. November 3-4, 2006.

"Structure Determination of Symmetric Homo-oligomers by a Complete Search of Symmetry Configuration Space Using NMR Restraints and van der Waals Packing" (with S. Potluri, A. Yan, J. Chou, and C. Bailey-Kellogg). 5th NIH/NIGMS Protein Structure Initiative "Bottlenecks" Workshop, Natcher Conference Center, NIH, Bethesda, Maryland. April 13-14, 2006.

"Molecular Symmetry as Aid to Homo-oligomeric Protein Structure Determination by NMR, using Sparse Inter-molecular NOE Restraints" (with S. Potluri and C. Bailey-Kellogg), Public Library of Science Computational Biology (PLoS CB) Late Breaking Posters, the International Conference on Intelligent Systems for Molecular Biology (ISMB), (June, 2005) Detroit, MI.

"High-Throughput 3D Homology Detection via NMR Resonance Assignment" (with C. Langmead), *Eighth Annual International Conference on Research in Computational Molecular Biology (RE-COMB),* San Diego (March 27-31, 2004). In *Currents in Computational Molecular Biology, 2004* (ed. A. Gramada and P. Bourne) p. 522.

A Probability-Based Similarity Measure for Saupe Alignment Tensors with Applications to Residual Dipolar Couplings in NMR Structural Biology (with A. Yan and C. Langmead) *Eighth Annual International Conference on Research in Computational Molecular Biology (RECOMB),* San Diego (March 27-31, 2004). In *Currents in Computational Molecular Biology, 2004* (ed. A. Gramada and P. Bourne) pp. 437-438.

A Framework for Automated NMR Resonance Assignments and 3D Structural Homology Detection (with C. Langmead). Gordon Conference on Computational Methods in Biomolecular NMR, Ventura, CA, January 18-23, 2004.

Exact Solutions for Internuclear Vectors and Dihedral Angles from Two RDCs and Their Application in a Systematic Search Algorithm for Determining Protein Backbone Structure (with L. Wang, R. Mettu, R. Lilien, and A. Yan). Gordon Conference on Computational Methods in Biomolecular NMR, Ventura, CA, January 18-23, 2004.

"An Exact Algorithm For Determining Protein Backbone Structure From NH Residual Dipolar Couplings," (with L. Wang, R. Mettu, and R. Lilien), *Proc. IEEE Computer Society Bioinformatics Conference (CSB)*, Stanford University, Palo Alto, (August 10, 2003) pp. 611-612. ISBN 0-7695-2000-6. (Refereed).

> Winner of Best Poster Award.

"Ensembles of active site conformations allow structure-based redesign and drug design," (with A. An-

derson, R. Lilien and V. Popov) 225th American Chemical Society National Meeting, March 23-28, 2003. New Orleans, LA.

"Modeling Protein Flexibility for Structure-Based Active Site Redesign," (with R. Lilien and A. Anderson) The Sixth Annual International Conference on Research in Computational Molecular Biology (RECOMB), Washington DC (2002). In *Currents in Computational Molecular Biology, 2002* (ed. L. Florea et al.) pp 122-123. (Refereed).

"Modeling of Protein Flexibility for Computational Active Site Redesign," (with R. Lilien and A. Anderson) the 16th Annual National MD/PhD Conference, Given Institute , Aspen, Colorado, July 13-15, 2001.

"Computational Screening Studies for Core-Binding Factor Beta (CBF-β): Use of Multiple Conformations to Model Receptor Flexibility," (with R. Lilien, M. Sridharan, X. Huang, and J. Bushweller), the 8th International Conference on Intelligent Systems for Molecular Biology (ISMB'2000), (August 20–23, 2000) La Jolla, CA.

"Time-Frequency Analysis of Protein NMR Data" (with C. J. Langmead), the 8th International Conference on Intelligent Systems for Molecular Biology (ISMB'2000), (August 20–23, 2000) La Jolla, CA.

"The NOESY Jigsaw: Automated Protein Secondary Structure and Main-Chain Assignment from Sparse, Unassigned NMR Data," (with C. Bailey-Kellogg, A. Widge, J. J. Kelley, III, M. J. Berardi, and J. H. Bushweller), the 8th International Conference on Intelligent Systems for Molecular Biology (ISMB'2000), (August 20–23, 2000) La Jolla, CA.

"Cooperating Autonomous Mobile Robots: Theory and Experiments," (with J. Jennings and D. Rus), NSF Design and Manufacturing Grantees Conference, MIT, Cambridge, MA (Jan. 1994)

14.11   Journal Issues

271. *Frontiers in Molecular Biosciences.* Editor for Special issue on Biological Modeling and Simulation, with Research Topic: Advances in Computational and Data-Driven Protein Design—Methods and Applications. Volume 9 (2023). DOI: tinyurl.com/37588d3k

272. *International Journal of Robotics Research*, Vol. 21 Issue 03, (2002) pp. 177–277. Guest Editor for special issue on *"Algorithmic Foundations of Robotics."*

273. *Algorithmica*, **(10),** Nos. 2/3/4, Aug/Sept/Oct (1993), pp. 91–352. Guest Editor for special issue on *"Computational Robotics: The Geometric Theory of Manipulation, Planning, and Control."*

274. *Algorithmica*, **(14),** No. 6 (1995) is devoted entirely to two of my papers (with P. Xavier).

14.12   Internally Refereed Reports

275. *Error Detection and Recovery for Robot Motion Planning with Uncertainty*, MIT Artificial Intelligence Laboratory, AI-TR-982, (1987).

276. *Simplified Voronoi Diagrams*, (with John Canny) MIT Artificial Intelligence Laboratory A.I. Memo 957, (1987)

277. *Motion Planning With Six Degrees of Freedom*, MIT Artificial Intelligence Laboratory AI-TR-791 (1984). (261 pp.) Based on S.M. thesis, "Local and Global Techniques for Motion Planning".

278. *Hypothesizing Channels Through Free-Space in Solving the Findpath Problem*, MIT Artificial Intelligence Laboratory A.I. Memo 736 (1983).

14.13   Theses and Dissertations

Ph.D. Thesis, Computer Science, Massachusetts Institute of Technology, 1987: *Error Detection and Recovery for Robot Motion Planning with Uncertainty.* Available from MIT AI Lab, MIT AI-TR-982 (`http://hdl.handle.net/1721.1/6851`)

S.M. Thesis, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, 1984: *Local and Global Techniques for Motion Planning.* Available from MIT AI Lab, MIT AI-TR-791 (`http://hdl.handle.net/1721.1/6944`) and MIT AI-TR-736 (`http://hdl.handle.net/1721.1/6393`)

B.A. Thesis, Russian Language and Literature, Yale University, 1980: *Blok, Esenin, and Post-Revolutionary Russia.*

14.14 Selected Other Papers

279. "OSPREY (Open Source Protein Redesign for You) User Manual – Version 2.2β" (with I. Georgiev K. Roberts, P. Gainza, and M. Hallen). Available online: www.cs.duke.edu/donaldlab/software.php (2009). Updated: 2010, 2012, and 2015. 97 pages.

280. "SAR by MS for Functional Genomics (Structure-Activity Relation by Mass Spectrometry)," (with C. Bailey-Kellogg, J. Kelley, and C. Stein), Dartmouth Computer Science Technical Report No. PCS-TR99-359, Hanover, NH, (October, 1999).

281. "Application Challenges to Computational Geometry", The Computational Geometry Impact Task Force Report, (with Chazelle, et al.) Technical Report TR-521-96, Princeton University, April 1996.

282. *How to do Research at the MIT AI Lab*, Working Paper 316, (with D. Chapman (ed.) et al.) MIT Artificial Intelligence Laboratory (1988).

283. *On The Complexity of Kinodynamic Planning*, Cornell Computer Science Department, Technical Report No. 88-929, (1988). (with J. Canny, J. Reif, and P. Xavier)

284. *A Geometric Approach to Error Detection and Recovery for Robot Motion Planning with Uncertainty*, Cornell Computer Science Department, Technical Report No. 88-895, (1988).

285. *On Planning: What is to be Done?*, Cornell Computer Science Department, Technical Report No. 87-890, (1987).

286. *The Complexity of Planar Compliant Motion Planning Under Uncertainty*, Cornell Computer Science Department, Technical Report No. 87-889, (1987).

287. *Planning Multi-Step Error Detection and Recovery Strategies*, Cornell Computer Science Department, Technical Report No. 87-880, (1987).

288. *Simplified Voronoi Diagrams*, Cornell Computer Science Department, Technical Report No. 87-879, (1987). (with John Canny).

289. *Towards Task-Level Robot Programming*, Cornell Computer Science Department, Technical Report No. 87-878, (1987).

290. *The EIGHT Manual: An Introduction to Geometric Modelling and Three-Dimensional Graphics on the Lisp Machine*, Working Paper 262, MIT Artificial Intelligence Laboratory (1984).

291. "A System for Computer-Aided Architectural Design: Computer-Aided Architecture at the Laboratory for Computer Graphics", This is the Technical Report for my presentation at the *Proc. Harvard Computer Graphics Conference* Cambridge, MA (July, 1982); see conference presentation # 202 above.

292. *Computing the Topology of 3-Dimensional Forms*, Laboratory for Computer Graphics and Spatial Analysis Geometric Modeling Series, Graduate School of Design, Harvard University (1981).

293. *Alternative Methods of Dynamic Language Creation: The* GLIB *Table-Driven Language Compiler*, Laboratory for Computer Graphics and Spatial Analysis, Graduate School of Design, Harvard University (1978).

294. *Random Number Generator for the* PDP-8/E, DECUSCOPE Digital Equipment Computer Users Society, Vol. 13, No. 1 (1974), pp. 11-13.

14.15 Exhibitions

295. *A Familiar Space in Two Dimensions* (Piper Auditorium Computer-aided Design (CAD) Study), (with Paul Stevenson Oles), Graduate School of Design, Harvard University (1982).