

Curriculum Vitæ

Bruce Randall Donald

William and Sue Gross Professor of Computer Science and Biochemistry
Duke University

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1 Principal Fields of Interest

Computational Molecular Biology.

Algorithms in Structural Molecular Biology.

Computational Chemistry.

Structural Genomics & Systems Biology.

Structural Biology & Biochemistry.

Microelectromechanical Systems (MEMS).

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: Artificial Intelligence Laboratory. Research supervisor: Professor Tomás Lozano-Pérez. Minor: Mathematics (Topology).

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

B.A. Yale University, 1980.

3 Professional Experience

(2006—) William and Sue Gross Professor of Computer Science, Duke University.

(2006—) Professor of Biochemistry, School of Medicine, Duke University Medical Center.

(2010—) Professor of Electrical and Computer Engineering, Pratt School of Engineering, 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.

(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

Finalist, NIH Director's Pioneer Award (2011).

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 (1985-7).

Graduated *Summa Cum Laude*, Yale University (1980).

Distinction in the Major, Yale University (1980).

Phi Beta Kappa, Yale University (1979).

Wallace Fiction Prize, Yale University (1978).
 J. E. Meeker Prize for Writing, Yale University (1977).

University Awards

Bass Society of Fellows, Duke University (2006–).
 Edward and Joan Foley Fellow, Dartmouth College (2000–2001).
 Senior Faculty Grant, Dartmouth College (2001).
 A.M. (Hon.) Dartmouth College, 2000.
 Friedman Faculty Fellow, Dartmouth College (1999–2000).

Distinguished and Inaugural Lectures

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).

Selected Best Paper/Poster Awards

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 §15.2.1). 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 Industry Experience and Consulting

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 §15.4, “Patents” and SIGGRAPH’2000 paper in §15.5).
 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

- Program committee, International Conference on Intelligent Systems for Molecular Biology (ISMB), Long Beach, CA. July 15-17, 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–).
- IEEE Fellows Nominations Committee, IEEE Robotics and Automation Society (March, 2011–).
- Program committee, International Conference on Intelligent Systems for Molecular Biology (ISMB), Vienna, Austria 2011.
- Program committee, International Conference on Intelligent Systems for Molecular Biology (ISMB), Boston, MA 2010.
- Senior Member, IEEE (2010).
- Invited Speaker, Northeastern Structure Symposium (NESS), University of Connecticut, Storrs. 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.
- Ad hoc* reviewer, 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.
- 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.
- Reviewer, MacArthur Fellows Program, The John D. and Catherine T. MacArthur Foundation (2003, 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.
- Ad hoc* reviewer, 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).
- Ad hoc* reviewer, 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).
- Moderator, Computing Research Repository — [arXiv.org](http://arxiv.org) e-Print archive, (Robotics) (1998 —).
- 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 Symposium 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 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).
- Reviewer/Referee for *PNAS*, *Proteins*, *PLoS Computational Biology*, *Protein Science*, *Jour. Am. Chem. Soc. (JACS)*, *PLoS One*, *Journal of Biomolecular NMR*, *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*, *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*, *Volkswagenstiftung*.

9 University Activities

9.1 Duke

University:

Provost's Advisory Committee on Promotions and Tenure (APT) Committee (2008–2009, 2010–).

Programs and Affiliations:

Computational Biology and Bioinformatics Ph.D. Program (2006–).
 Institute for Genome Sciences and Policy (IGSP), (2006–)
 Structural Biology and Biophysics Ph.D. Program (2007–).
 Cell and Molecular Biology Ph.D. Program (2008–).
 Duke Institute for Brain Sciences (DIBS) Faculty, (2008–),
 Duke Institute for Brain Sciences (DIBS) Investigator, (2008–),

Computer Science Department:

Executive committee (2006–).
 Tenure committee (member: 2006-7, 2010-11; chair: 2007-8).
 Reappointment committee (member: 2008).
 Promotion committee (chair: 2009).
 Committee to Write the 10-year Strategic Plan (member: 2009).
 Faculty Search Committee (2006-8).
 Graduate committee (2006-8, 2010-11).
 6 RIP (“Research in Progress”) Graduate Committees (2006–).

Biochemistry Department:

Computer and Shared Resources Committee (2006–).

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–).

IGSP

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

9.2 Dartmouth

Ad Hoc 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**

“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

Lectures and Colloquia: 1996–present

“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 Presentation, 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, Storrs. 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, $250 \times 60 \mu\text{m}$ 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, 21st Conference on Uncertainty in Artificial Intelligence (UAI), University of Edin-
burgh, 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, Department 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.
 - Computer Science Department, 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).

Lectures and Colloquia: 1986-1995

- 1995** Princeton; CMU; UCLA; Interval Research Corp.
- 1994** SRI; Xerox PARC; Dartmouth; Berkeley; Stanford; Wright-Patterson Air Force Base.
- 1993** WAFR'93; NSF; Air Force Office of Sponsored Research (AFOSR); AFOSR Electronic Prototyping Grantees Review Meeting; Workshop on Geometric Algorithms for Manufacturing, IEEE Int. Conf. on Robotics and Automation; AAAI Workshop on Computational Theories of Interaction and Agency, University of Chicago; AAAI Fall Symposium Series.
- 1992** International Symposium on Symbolic and Algebraic Computation (ISSAC), Workshop on Integrated Symbolic-Numeric Computing, Berkeley, CA; University of Illinois at Urbana-Champaign (UIUC) (two lectures).
- 1991** Stanford; 1st AAAI Fall Symposium on Sensory Aspects of Robotic Intelligence, Asilomar, CA; University of Chicago.
- 1990** NYU Courant; CMU; Princeton; United Parcel Service Research and Development; Yale; Saratoga Workshop on the Integration of Numerical and Symbolic Computing Methods, Saratoga, NY; Xerox PARC (three lectures); Wright-Patterson Air Force Base; American Mathematical Society, Louisville, Kentucky.
- 1989** AT&T Bell Labs; Oxford University; I.R.S.T (Istituto per la Ricerca Scientifica e Tecnologica), Istituto Trentino di Cultura, Trento, Italy (4 lectures); CMU; Northwestern; MIT; Stanford; Panel on Robot Autonomy and Dexterity, NASA Conference on Space Telerobotics, Jet Propulsion Laboratory, California Institute of Technology.
- 1986-8** Duke; Berkeley; NYU Courant; US/France Workshop on Automatic Robot Programming, MIT; CMU; UIUC; Cornell; University of Wisconsin (Madison); U.S.C; Caltech; IBM Watson Research Center.

12 Students and Post-Docs Currently Supervised

12.1 Current Post-Docs

Stuart Endo-Streeter (2009–)

Michael Zeng (2011–)

12.2 Thesis Advisor, Current Ph.D Students

John MacMaster, Computer Science Department, Duke University.

Chittaranjan Tripathy, Computer Science Department, Duke University.

Cheng-Yu Chen, Biochemistry Department, Duke University Medical Center.

Kyle Roberts, Computational Biology, Duke University Medical Center.

Jeffrey Martin, Computer Science Department, Duke University.

Swati Jain, Program in Computational Biology and Bioinformatics, Duke University Medical Center.

Mark Hallen, Biochemistry Department, Duke University Medical Center.

Pablo Gainza, Computer Science Department, Duke University.

Inho Yoon, Department of Electrical and Computer Engineering, Pratt School of Engineering, Duke University.

12.3 Thesis Reader: PhD

Pre-doctoral (Current)

Dan Keedy, Department of Biochemistry, Duke University Medical Center.

Himanshu Chandola, Dartmouth CS.

13 Students and Post-Docs Supervised

13.1 Post-Docs

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.)

Jonathan Rees (1991-92). (First job: Sussex/MIT. Now lead scientist at Millennium Pharmaceuticals on the pathways database project).

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).

John J. Kelley III (1999–2001). (Now at the University of Michigan).

Christopher Bailey-Kellogg (1999–2001). (First Job: Assistant Professor of Computer Science at Purdue. Now Assistant Professor of Computer Science at Dartmouth).

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).

Tae-Cheon Yang (2003–2004). (Now Associate Professor of Computer Science, Kyungsung University, Korea.)

Ram Mettu (2002–2005). (First job: Assistant Professor of Electrical and Computer Engineering at the University of Massachusetts, Amherst. Now at the Department of Computer Science, Tulane University).

Rahul Ray (2004-2006). (First job: Assistant Professor of Computer Science at IIT-Madras).

Ryan Lilien (2004-2006) is listed in §13.2.1.

Serkan Apaydin (2004–2008)

Now on Faculty of Engineering and Sciences at Sabanci University in Istanbul, Turkey.

Nanjiang Shu (2008–2009)

Now at Boston University.

Anna Yershova (2008–2011).

Now at the University of Illinois at Urbana-Champaign.

13.2 Thesis Advisor (Ph.D)

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 is now a Senior Member of the Technical Staff at Sandia National Labs.

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.

Russell Brown, *Localization, Mapmaking, and Distributed Manipulation with Flexible, Robust Mobile Robots*. PhD (February 1995) Computer Science Department, Cornell University.

Dr. Brown is now a Senior Member of the Technical Staff at Sandia National Labs.

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 Department for the ACM Distinguished Dissertation Award.

Dr. Böhringer is now an full Professor of Electrical Engineering at the University of Washington (U.W.), Seattle, and director of the U.W. MEMS Laboratory.

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 at IBM.

Chris Langmead, *Molecular Replacement for Nuclear Magnetic Resonance: Application to NMR Resonance Assignment and Protein Structure Determination*. Ph.D. (2003) Computer Science Department, Dartmouth College.

Dr. Langmead is now an Assistant Professor of Computer Science at Carnegie-Mellon University.

Ryan Lilien (Ph.D., 2004) is listed in §13.2.1.

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).

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.

Dr. Paprotny is currently a research faculty member at The Berkeley Sensors and Actuator Center (BSAC), U.C. Berkeley.

Anthony K. Yan, *Geometric Methods for NMR Structure Determination of Symmetric Homo-oligomers*, Ph.D. (2008) Computer Science Department, Dartmouth College.

Dr. Yan is currently a postdoc in the laboratory of Dr. Pei Zhou, Duke Biochemistry Department.

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 is currently co-head of the Structural Bioinformatics Section at the Vaccine Research Center, NIAID, NIH.

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 is currently a postdoc in the laboratory of Peter M. Glazer, Department of Therapeutic Radiology, Yale University School of Medicine.

Michael Zeng, *Novel Algorithms for Automated NMR Assignment and Protein Structure Determination*, Ph.D. (2011) Department of Computer Science, Duke University.

13.2.1 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.

13.3 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).

13.4 Senior Theses Supervised

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.

13.5 Advisor, Undergraduate Independent Study (Selected List)

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

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.

13.6 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), *C² 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.

13.7 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.

14 Research Grants and Contracts

- (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.
- (2008–2013) *Computational Active-Site Redesign and Binding Prediction via Molecular Ensembles*, National Institutes of Health, National Institute of General Medical Sciences (NIGMS) (R01 GM-078031) \$1,257,125.
- (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.
- (2002–2007) Initial application 1R01 GM-65982, \$1,211,813. NIGMS Protein Structure Initiative.
- (2007–2012) Competing renewal 2R01 GM-65982, \$1,209,668.
- (2009–2011) ARRA Supplement, 3R01 GM-65982-08S1, \$262,516.
- (2005–2010) *Bioinformatics and Computational Biology Training Program*. National Institutes of Health, National Institute of General Medical Sciences (T32 GM-71340), \$1,079,891.
- (2005–2010) Initial application 1T32 GM-71340, \$899,175.
- (2009–2010) ARRA Supplement, 3T32 GM-71340-05S1, \$180,716.
- (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.
- (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, \$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 (PVI) 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.

15 List of Publications

15.1 Books

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

15.2 Papers in Refereed Journals

15.2.1 Structural Molecular Biology and Biochemistry

- “Protein Loop Closure Using Orientational Restraints from NMR Data,” (with C. Tripathy, J. Zeng, and P. Zhou). *Proteins: Structure, Function, and Bioinformatics* (2011) in press. Epub ahead of print: DOI: 10.1002/prot.23207
- “A Graphical Method for Analyzing Distance Restraints using Residual Dipolar Couplings for Structure Determination of Symmetric Protein Homoöligomers” (with J. Martin, A. Yan, C Bailey-Kellogg, and P. Zhou). *Protein Science* 20(6):970–985 (2011). Mar 16. doi: 10.1002/pro.620. [Epub ahead of print]
- “Predicting Resistance Mutations using Protein Design Algorithms” (with K. Frey, I. Georgiev, and A. Anderson). *Proceedings of the National Academy of Sciences, U.S.A. (PNAS)* 2010; 107(31):13707–13712.
- “High-Resolution Protein Structure Determination 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). *Journal of Biomolecular NMR* 2009; 45(3):265–281.
- “Computational Structure-Based Redesign of Enzyme Activity” (with C.-Y. Chen, I. Georgiev, and A. Anderson). *Proceedings of the National Academy of Sciences, U.S.A. (PNAS)* 2009; 106(10):3764–3769.
- “Automated NMR Assignment and Protein Structure Determination using Sparse Dipolar Coupling Constraints” (with J. Martin). *Progress in NMR Spectroscopy* 2009; 55(2):101–127.
- “Allosteric Inhibition of the Protein-Protein Interaction Between the Leukemia-Associated Proteins RUNX1 and CBF β ” (with M. Gorczyński, J. Grembecka, Y. Zhou, Y. Kong, L. Roudaiya, M. Douvas, M. Newman, I. Bielnicka, G. Baber, T. Corpora, J. Shi, M. Sridharan, R. Lilien, N. Speck, M. Brown, and J. Bushweller). *Chemistry & Biology* 2007; 14(10):1186–1197. Cover Article.
- “Redesigning the PheA Domain of Gramicidin Synthetase Leads to a New Understanding of the Enzyme’s Mechanism and Selectivity” (with B. Stevens, R. Lilien, I. Georgiev, and A. Anderson). *Biochemistry* 2006; 45(51):15495–15504.
- “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). *Proteins: Structure, Function, and Bioinformatics* 2006; 65(1):203–219.
- “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), *Journal of Computational Biology* 2005; 12(6-7):740–761.
- “Phylogenetic Classification of Protozoa Based on the Structure of the Linker Domain in the Bifunctional Enzyme, Dihydrofolate Reductase-Thymidylate Synthase,” (with R. O’Neil, R. Lilien, R. Stroud, and A. Anderson) *Journal of Biological Chemistry* 2003; 278(52):52980–52987.
- “The Crystal Structure of Dihydrofolate Reductase-Thymidylate Synthase from *Cryptosporidium hominis* Reveals a Novel Architecture for the Bifunctional Enzyme,” (with R. O’Neil, R. Lilien, R. Stroud, and A. Anderson) *Journal of Eukaryotic Microbiology* 2003; 50(6):555–556. Cover article.

15.2.2 Computational Molecular Biology and Computational Chemistry

- “Protein Design using Continuous Rotamers,” (with P. Gainza and K. Roberts). *PLoS Computational Biology* (2011) In Press.
- “Protein Side-Chain Resonance Assignment and NOE Assignment Using RDC-Defined Backbones without TOCSY Data,” (with J. Zeng and P. Zhou). *Journal of Biomolecular NMR* 2011; **50**:371–395.
- “NMR Structural Inference of Symmetric Homo-Oligomers” (with H. Chandola, A. Yan, S. Potluri, and C. Bailey-Kellogg). *Journal of Computational Biology* 2011; 18(12):1757–75. PMID: 21718128.
- “A geometric arrangement algorithm for structure determination of symmetric protein homo-oligomers from NOEs and RDCs,” (with J. Martin, A. Yan, C. Bailey-Kellogg, and P. Zhou). *Journal of Computational Biology* 2011; 18(11):1507–23.
- “A Bayesian Approach for Determining Protein Side-chain Rotamer Conformations using Unassigned NOE Data” (with J. Zeng, K. Roberts, and P. Zhou). *Journal of Computational Biology* 2011; 18(11):1661–79.
- “NVR-BIP: Nuclear Vector Replacement using Binary Integer Programming for NMR Structure-Based Assignments” (with S. Apaydin, B. Catay, and N. Patrick). *The Computer Journal* 2011; **54**:708–716. Epub online in summer 2010.
- Algorithm for Backrub Motions in Protein Design (with I. Georgiev, D. Keedy, J. Richardson, and D. Richardson). *Bioinformatics* 2008; 24(13):i196–i204.
- “Structure-Based Protein NMR Assignments using Native Structural Ensembles,” (with S. Apaydin and V. Conitzer). *Journal of Biomolecular NMR* 2008; 40(4):263–276.
- “The 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). *Journal of Computational Chemistry* 2008; 29(10):1527–42.
- “Dead-End Elimination with Backbone Flexibility” (with I. Georgiev), *Bioinformatics* 2007; 23(13):i185–i194.
- “A Complete Algorithm to Resolve Ambiguity for Inter-subunit NOE Assignment in Structure Determination of Symmetric Homo-oligomers,” (with S. Potluri, A. Yan, and C. Bailey-Kellogg). *Protein Science* 2007; 16(1):69–81.
- “A polynomial-time algorithm for *de novo* protein backbone structure determination from NMR data,” (with L. Wang and R. Mettu). *Journal of Computational Biology* 2006; 13(7): 1276–1288.
- “Improved Pruning Algorithms and Divide-and-Conquer Strategies for Dead-End Elimination, with Application to Protein Design” (with I. Georgiev and R. Lilien), *Bioinformatics* 2006; **22**(14):e174–183.
- “High-Throughput Inference of Protein-Protein Interfaces from Unassigned NMR Data” (with R. Mettu and R. Lilien), *Bioinformatics* 2005; **21**(Suppl. 1):i292–i301.
- “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), *The International Journal of Robotics Research* Special Issue on Robotics Techniques Applied to Computational Biology 2005; (29)(**2–3**):165–182.
- “Exact Solutions for Internuclear Vectors and Backbone Dihedral Angles from NH Residual Dipolar Couplings in Two Media, and Their Application in a Systematic Search Algorithm for Determining Protein Backbone Structure” (with L. Wang), *Journal of Biomolecular NMR* 2004; 29(**3**):223–242.
- “An Expectation/Maximization Nuclear Vector Replacement Algorithm for Automated NMR Resonance Assignments” (with C. Langmead), *Journal of Biomolecular NMR* 2004; 29(**2**):111–138.
- “A Polynomial-Time Nuclear Vector Replacement Algorithm for Automated NMR Resonance Assignments,” (with C. Langmead, A. Yan, R. Lilien, and L. Wang) *Journal of Computational Biology* 2004; 11(**2–3**):277–298.
- “A Subgroup Algorithm to Identify Cross-Rotation Peaks Consistent with Non-Crystallographic Symmetry” (with R. Lilien, C. Bailey-Kellogg, and A. Anderson). *Acta Crystallographica D: Biological Crystallography* 2004; **D60**, 1057–1067.
- “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) *Journal of Computational Biology* 8(**1**):19–36, 2001.
- “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), *Journal of Computational Biology*, 7(3-4) (2000) pp. 537–558.

15.2.3 Systems Biology

“Probabilistic Disease Classification of Expression-Dependent Proteomic Data from Mass Spectrometry of Human Serum,” (with R. Lilien and H. Farid), *Journal of Computational Biology*, 10(6) 2003 pp. 925–946.

“Phase-Independent Rhythmic Analysis of Genome-Wide Expression Patterns”, (with C. Langmead, A. Yan, and C. R. McClung), *Journal of Computational Biology* 10(3-4) 2003, pp. 521-536.

Note: Some papers in § 15.2.1– 15.2.2 also relate to Systems Biology.

15.2.4 Microelectromechanical Systems (MEMS)

“Planar Microassembly by Parallel Actuation of MEMS Microrobots” (with C. Levey and I. Paprotny). *Journal of Microelectromechanical Systems* 2008; 17(4):789–808.

“An Untethered, Electrostatic, Globally-Controllable MEMS Micro-Robot” (with C. Levey, C. McGray, I. Paprotny, and D. Rus), *Journal of Microelectromechanical Systems* 2006; 15(1):1–15.

“Power Delivery and Locomotion of Untethered Micro-Actuators,” (with C. Levey, C. McGray, D. Rus, and M. Sinclair), *Journal of Microelectromechanical Systems*, (2003) 10(6):947–959.

“Part Orientation with One or Two Stable Equilibria Using Programmable Vector Fields,” (with K.-F. Böhringer, F. Lamiraux, and L. Kavraki), *IEEE Transactions on Robotics and Automation*, 16(2), April 2000, pp. 157-170.

“Sensorless Manipulation Algorithms Using a Vibrating Surface,” (with K.-F. Böhringer, V. Bhatt, and K. Goldberg) *Algorithmica*, 26(3/4), March/April (2000). Special Issue on Algorithmic Foundations of Robotics, pp. 389–429.

“CMOS Integrated Organic Ciliary Array for General-Purpose Micromanipulation Tool for Small Objects,” (with J. Suh, R. B. Darling, K.-F. Böhringer, H. Baltes, and G. Kovacs), *Journal of Microelectromechanical Systems*, vol. 8, No. 4 (Dec. 1999), pp. 483–496.

“Programmable Vector Fields for Distributed Manipulation, with Applications to MEMS Actuator Arrays and Vibratory Parts Feeders,” (with K.-F. Böhringer and N. C. MacDonald), *International Journal of Robotics Research*, vol. 18(2), February, 1999 pp. 168–200.

“Computational Methods for the Design and Control of MEMS Micromanipulator Arrays,” (with K.-F. Böhringer, N. MacDonald, G. Kovacs, and J. Suh), *IEEE Computational Science and Engineering*, Vol. 4, No. 1. Special Issue on Computational MEMS, pp. 17–29. Jan-March 1997.

15.2.5 Robotics and Motion Planning

“Visibility-Based Planning of Sensor Control Strategies,” (with A. J. Briggs), *Algorithmica*, 26(3/4), March/April (2000), pp. 364–388.

“Mobile Robot Self-Localization without Explicit Landmarks,” (with R. G. Brown), *Algorithmica*, Special Issue on Algorithmic Foundations of Robotics 26(3/4), March/April (2000), pp. 515–559.

“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.

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

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

“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.

“Provably Good Approximation Algorithms for Optimal Kinodynamic Planning: Robots with Decoupled Dynamics Bounds” (with P. Xavier) *Algorithmica*, (14), No. 6 (1995) pp. 480-530.

“Kinodynamic Motion Planning”, (with P. Xavier, J. Canny, and J. Reif) *Journal of the ACM*, Vol. 40, No. 5, Nov., 1993. pp. 1048-1066.

- “Constructive Recognizability for Task-Directed Robot Programming”, (with J. Jennings), *Jour. Robotics and Autonomous Systems*, **(9)**, No. 1, Elsevier/North-Holland (1992). (Invited). pp. 41-74.
- “Computational Robotics: Manipulation, Planning, and Control”, *Algorithmica* Vol. 10, Nos. 2/3/4, Aug/Sept/Oct. 1993 (Editor’s introduction).
- “The Motion of Planar Compliantly-Connected Rigid Bodies in Contact, with Applications to Automatic Fastening,” (with D. Pai), *International Journal of Robotics Research* **12**, (4), August 1993, pp. 307-338.
- “Robot Motion Planning, ” *IEEE Trans. on Robotics and Automation*, **(8)**, No. 2. April, 1992. (Invited book review).
- “On Planning: What is to be Done?”, *Communication and Cognition—Artificial Intelligence*, Special Issue on AI and Robotics, Vol. 9. No. 1 (Invited) (1992) pp. 89-132
- “Planning Multi-Step Error Detection and Recovery Strategies”, *International Journal of Robotics Research*, **9** (1), Feb. 1990. pp. 3-60.
- “The Complexity of Planar Compliant Motion Planning with Uncertainty”, *Algorithmica*, **5** (3), 1990 pp. 353-382.
- “A Geometric Approach to Error Detection and Recovery for Robot Motion Planning with Uncertainty”, *Artificial Intelligence*, **37** (1-3), Dec. 1988. pp. 223-271.
- “A Search Algorithm for Motion Planning with Six Degrees of Freedom”, *Artificial Intelligence* **31** (3), 1987. pp. 295-353.

15.2.6 Computational Geometry

- “On the Area Bisectors of a Polygon,” (with K.-F. Böhringer and D. Halperin) *Discrete and Computational Geometry*, vol. 22 (1999), pp. 269–285.
- “Simplified Voronoi Diagrams”, (with John Canny) *Discrete and Computational Geometry*, **3** (3), 1988. pp. 219-236.

15.3 Protein Structures

- Solution structure of the FF Domain 2 of human transcription elongation factor CA150, (with M. Zeng, C. Tripathy, J. Boyles, A. Yan, and P. Zhou), PDB ID: 2KIQ (2009).
- Complete ensemble of NMR structures of Unphosphorylated Human Phospholamban Pentamer, (with S. Potluri, A. Yan, J. Chou, and C. Bailey-Kellogg), PDB ID: 2HYN (2006).
- Crystal structure of Dihydrofolate Reductase-Thymidylate Synthase (DHFR-TS) from *Cryptosporidium hominis*, (with R. O’Neil, R. Lilien, R. Stroud, and A. Anderson), PDB ID: 1QZF (2003).

15.4 Patents

- 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.

15.5 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.

15.5.1 Computational Molecular Biology

Algorithms in Structural Molecular Biology

- “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 43/153 acceptance rate.
- “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 43/153 acceptance rate.
- “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 43/153 acceptance rate.
- “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 43/153 acceptance rate.
- “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). 25/60 acceptance rate.
- “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. < 36/175 acceptance rate.
- “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.
- “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).
- “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. 30/135 acceptance rate.
- “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).
- “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. 30/156 acceptance rate.

Winner of Best Paper Award.

- “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).
- “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.
- “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. 40/212 acceptance rate.
- “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. 30/264 acceptance rate.
- “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. 38/264 acceptance rate.
- “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) 56/428 acceptance rate.
- “Computational and physical modeling challenges in structural molecular biology and proteomics,” *ACM Symposium on Solid and Physical Modeling 2005*: 7. Invited.
- “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).
- “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). 41/202 acceptance rate.
- “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). 41/202 acceptance rate.
- “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. 38/215 acceptance rate.
- “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. 36/151 acceptance rate.
- “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. 35/175 acceptance rate.
- “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. 35/128 acceptance rate.
- “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. 40/140 acceptance rate.

“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.

“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.

Systems Biology

“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: 19/103.

“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: 35/118.

Note: Some papers in § 15.5.1 also relate to Systems Biology.

15.5.2 Microelectromechanical Systems (MEMS)

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

“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.

“A Steerable, Untethered, $250 \times 60 \mu\text{m}$ 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.

“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.

“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.

“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.

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

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

“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.

“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.

“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).
- “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).
- “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).
- “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).

15.5.3 Computer Graphics and Haptics

- “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.
- “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.
- “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.

15.5.4 Robotics and Motion Planning

- “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.
- “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.
- “Experiments in Constrained Prehensile Manipulation: Distributed Manipulation with Ropes,” (with L. Gariepy and D. Rus) *International Symposium on Experimental Robotics (ISER)*, Sydney, Australia (1999).
- “Robust geometric algorithms for sensor planning,” (with A. Briggs), *International Workshop on the Algorithmic Foundations of Robotics (WAFR)*, Toulouse, France, July 1996.
- “Moving Furniture with Teams of Autonomous 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.
- “Distributed Robotic Manipulation: Experiments in Minimalism,” *International Symposium on Experimental Robotics*, Stanford, CA (1995).
- “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).
- “Automatic Sensor Configuration for Task-Directed Planning,” (with A. J. Briggs), *Proc. IEEE International Conference on Robotics and Automation*, San Diego, CA (May, 1994).
- “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).
- “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).
- “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).
- “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*. Chambéry, France (Aug 28, 1993).

- “Information Invariants in Robotics: Part I – State, Communication, and Side-Effects,” *Proc. IEEE International Conference on Robotics and Automation*, Atlanta, May (1993).
- “Information Invariants in Robotics: Part II – Sensors and Computation,” *Proc. IEEE International Conference on Robotics and Automation*, Atlanta, May (1993).
- “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.
- “Program Mobile Robots in Scheme,” (with J. Rees) *Proc. IEEE International Conference on Robotics and Automation*, Nice, France (May, 1992), pp. 2681-2688.
- “Programming Autonomous Agents: A Theory of Perceptual Equivalence” (with J. Jennings), 1st AAAI Fall Symposium on Sensory Aspects of Robotic Intelligence, Asilomar, CA (Nov, 1991). (Invited)
- “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.
- “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.
- “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.
- “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*, Cincinnati, Ohio (May 1990) pp. 1756–1763.
- “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.
- “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.
- “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.
- “Planning Multi-Step Error Detection and Recovery Strategies”, *Proc. IEEE International Conference on Robotics and Automation*, Philadelphia, PA April, 1988, pp. 892-897.
- “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).
- “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).
- “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).
- “The Mover’s Problem in Automated Structural Design”, *Proc. Harvard Computer Graphics Conference*, Cambridge, MA 1983, (Invited).

15.5.5 Computational Geometry

- 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.
- “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.
- “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.
- “On the Complexity of Computing the Homology Type of a Triangulation”, (with D. Chang), *IEEE Sym-*

- posium on the Foundations of Computer Science*, San Juan, (October 1991), pp. 650-661.
- “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.
- “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.
- “The Complexity of Planar Compliant Motion Planning with Uncertainty”, *Proc. 4th ACM Symposium on Computational Geometry*, Urbana, IL June, 1988, pp. 309-318.
- “Simplified Voronoi Diagrams”, (with John Canny) *Proc. Third ACM Symposium on Computational Geometry*, Waterloo, Ontario (June 1987), pp. 153-161.

15.6 Articles and Chapters in Multiply-Authored Books

- “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.
- “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.
- “A Steerable, Untethered, $250 \times 60 \mu\text{m}$ 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 Tracts in Advanced Robotics 28, Ed. S. Thrun *et al.*. Springer-Verlag (Berlin) 2007 pp. 337–356.
- “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.
- “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.
- “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.
- “A Single Universal Force Field Can Uniquely Orient Non-symmetric Parts,” (with K.-F. Böhringer, F. Lamiroux, and L. Kavraki), in *Robotics Research*, eds. J. Hollerbach and D. Koditschek, Springer-Verlag (London) 2000, pp. 395–402.
- “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.
- “A Distributed, Universal Device for Planar Parts Feeding: Unique Part Orientation in Programmable Force Fields,” (with K.-F. Böhringer, F. Lamiroux, and L. Kavraki), in *Distributed Manipulation*, ed. K. Böhringer *et al.*, Kluwer Academic Publishing (2000), pp. 1–28.
- “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.
- “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.
- “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.
- “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.
- “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.
- “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.
- “On Information Invariants in Robotics,” in *Computational Theories of Interaction and Agency*, MIT Press (1996), ed., P. Agre and S. Rosenschein.
- “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.
- “A Geometric Approach to Error Detection and Recovery for Robot Motion Planning with Uncertainty”, in *Geometric Reasoning*, MIT Press, Cambridge (1989), pp. 223-274.
- “Simplified Voronoi Diagrams”, (with John Canny), in *Autonomous Robot Vehicles*, Springer-Verlag, New York: (1990), pp. 272-289.
- “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.

15.7 Selected Invited Papers

- “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.
- “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.
- “Prototyping Animation Motion Control with Haptic Programmable Force Fields”, Workshop on “Motion Support in Virtual Prototyping,” (with Fred Henle) Stanford, May 5-7, 1999.
- “CMOS Integrated Organic Ciliary Array as a General-Purpose Micromanipulation Tool,” (with J. Suh, R. B. Darling, K.-F. Böhringer, H. Baltés, and G. Kovacs), IEEE International Conference on Robotics and Automation, Workshop on Distributed Manipulation (Detroit) May 11, 1999.
- “Part Orientation with One or Two Stable Equilibria Using Programmable Vector Fields,” (with K.-F. Böhringer, F. Lamiroux, and L. Kavraki), IEEE International Conference on Robotics and Automation, Workshop on Distributed Manipulation (Detroit) May 11, 1999.
- “Experiments in Constrained Prehensile Manipulation: Distributed Manipulation with Ropes,” (with L. Gariépy and D. Rus) IEEE International Conference on Robotics and Automation, Workshop on Distributed Manipulation (Detroit) May 11, 1999.
- “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).

15.8 Selected Conference Abstracts and Posters

- “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, July 2010. (Selected for Oral Presentation).
- “NMR structural inference of symmetric homo-oligomers” (with H. Chandola and C. Bailey-Kellogg). Structural Bioinformatics and Computational Biophysics (3DSIG), ISMB Satellite Meeting, Boston, 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 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). 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.
- “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).
- ”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. Apaydin 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. Apaydm). 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.
- “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.
- “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 (RECOMB)*, 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. (Referred).
- Winner of Best Poster Award.

- “Ensembles of active site conformations allow structure-based redesign and drug design,” (with A. Anderson, 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)

15.9 Journal Issues

- International Journal of Robotics Research*, Vol. 21 Issue 03, (2002) pp. 177–277. Guest Editor for special issue on “*Algorithmic Foundations of Robotics.*”
- 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.*”
- Algorithmica*, (14), No. 6 (1995) is devoted entirely to two of my papers (with P. Xavier).

15.10 Internally Refereed Reports

- Error Detection and Recovery for Robot Motion Planning with Uncertainty*, MIT Artificial Intelligence Laboratory, AI-TR-982, (1987).
- Simplified Voronoi Diagrams*, (with John Canny) MIT Artificial Intelligence Laboratory A.I. Memo 957, (1987)
- 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”.
- Hypothesizing Channels Through Free-Space in Solving the Findpath Problem*, MIT Artificial Intelligence Laboratory A.I. Memo 736 (1983).

15.11 Theses

- Ph.D** thesis, Computer Science, Massachusetts Institute of Technology, 1987: *Error Detection and Recovery for Robot Motion Planning with Uncertainty.*
- S.M.** thesis, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, 1984: *Local and Global Techniques for Motion Planning.*

15.12 Selected Other Papers

- “OSPREY (Open Source Protein Redesign for You) User Manual” (with I. Georgiev). Available online: www.cs.duke.edu/donaldlab/software.php (2009). Updated, 2010. 77 pages.

- “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).
- “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.
- On The Complexity of Kinodynamic Planning*, Cornell Computer Science Department, Technical Report No. 88-929, (1988). (with J. Canny, J. Reif, and P. Xavier)
- A Geometric Approach to Error Detection and Recovery for Robot Motion Planning with Uncertainty*, Cornell Computer Science Department, Technical Report No. 88-895, (1988).
- On Planning: What is to be Done?*, Cornell Computer Science Department, Technical Report No. 87-890, (1987).
- The Complexity of Planar Compliant Motion Planning Under Uncertainty*, Cornell Computer Science Department, Technical Report No. 87-889, (1987).
- Planning Multi-Step Error Detection and Recovery Strategies*, Cornell Computer Science Department, Technical Report No. 87-880, (1987).
- Simplified Voronoi Diagrams*, Cornell Computer Science Department, Technical Report No. 87-879, (1987). (with John Canny).
- Towards Task-Level Robot Programming*, Cornell Computer Science Department, Technical Report No. 87-878, (1987).
- The EIGHT Manual: An Introduction to Geometric Modelling and Three-Dimensional Graphics on the Lisp Machine*, Working Paper 262, MIT Artificial Intelligence Laboratory (1984).
- “A System for Computer-Aided Architectural Design: Computer-Aided Architecture at the Laboratory for Computer Graphics”, *Proc. Harvard Computer Graphics Conference* Cambridge, MA (July, 1982).
- Computing the Topology of 3-Dimensional Forms*, Laboratory for Computer Graphics and Spatial Analysis Geometric Modeling Series, Graduate School of Design, Harvard University (1981).
- 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).
- Random Number Generator for the PDP-8/E*, DECUSCOPE Digital Equipment Computer Users Society, Vol. 13, No. 1 (1974), pp. 11-13.

15.13 Exhibitions

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