

Robert L. Jernigan

Baker Center for Bioinformatics and Computational Biology
Plant Sciences Institute
112 Office and Laboratory Building
Iowa State University
Ames, Iowa 50011-3020
515-294-3833

Education

- 1963* – B.S. in Chemistry, California Institute of Technology
- 1968* – Ph.D. in Chemistry, Stanford University
Thesis on Statistical Mechanics of Polymers.
Advisor: P. J. Flory (Nobel Laureate)
- 1968* – Postdoctoral Fellow, Stanford University, with P. J. Flory
- 1968 – 1970* NIH Postdoctoral Fellow, University of California, San Diego, with B. H. Zimm
- 1970 – 1974* Senior Staff Fellow, Physical Sciences Laboratory, Division of Computer Research and Technology, National Institutes of Health
- 1974 – 1975* Senior Staff Fellow, Laboratory of Theoretical Biology, National Cancer Institute, National Institutes of Health

Professional Positions

- 1975 – 2002* Physical Chemist, Laboratory of Experimental and Computational Biology, National Cancer Institute, National Institutes of Health
- 1989 – 2002* Deputy Chief, Laboratory of Experimental and Computational Biology
- 1992 – 2002* Chief, Section on Molecular Structure
- 2002 – Pres.* Director, Laurence H. Baker Center for Bioinformatics and Biological Statistics, Iowa State University
- 2002 – Pres.* Professor, Department of Biochemistry, Biophysics and Molecular Biology, Iowa State University

Committees

- 1984 – 1988* Chairman, NIH Advisory Committee on Computer Usage
- 1989 – 2002* Time Allocation Group for supercomputer time at the Advanced Scientific Computing Laboratory, FCRDC, Frederick
- 1989 – 2002* NCI-Advanced Scientific Computing Laboratory Coordination Group
- 1993 – 1998, 2000 – 2002* NIH Inter-Institute Structural Biology Steering Group

1993 – 2002 Resource Advisory Committee for Parallel Processing Resource, Cornell University Theory Center

1994 – Award Committee - Biophysical Society

1995 – 1997 NIH Telecommunications Committee

2001 – *Pres.* Publications Committee, Biophysical Society overseeing Biophysical Journal

2003 – *Pres.* Chairman, Publications Committee, Biophysical Society

2002 – *Pres.* Plant Sciences Institute Council, Iowa State University

2002 – *Pres.* Supervisory Committee, Bioinformatics and Computational Biology Program

2003– *Pres.* Biochemistry, Biophysics and Molecular Biology Department - Computing Committee

2005 – National Advisory, Minnesota Supercomputing Institute, Univ. Minn.

2005 – *Pres.* - External Advisory Committee, Tuskegee University (NSF HBCU-HP)

2004 – *Pres.* - Departmental Promotion and Tenure Committee

2007 - Research Computing Council (ISU)

2008 - Program Committee for Intelligent Systems for Molecular Biology

2008 - Program Committee for European Conference on Computational Biology

2009 – Program Committee International Society for Computational Biology, Stockholm

Current - Program of Study committees – 25 graduate students

Professional Memberships

American Association for the Advancement of Science
 American Chemical Society
 Biophysical Society
 Protein Society
 American Society for Biochemistry and Molecular Biology
 International Society for Computational Biology

Current editorial boards

Biochemistry
 Journal of Biological Chemistry
 Bioinformatics and Biological Insights

Awards

NIH Special Achievement Cash Award 1982

Grant from NIH Intramural Targeted Anti-Viral AIDS Program for "Calculations of Preferred Ligands of the HIV-1 Protease Surface", 1990-1 and 1991-2

Grant from NIH Intramural Targeted Anti-Viral AIDS Program for "Enzyme Binding Sites for Peptides", 1992-3; 1993-1994

Grant from United States-Israel Binational Science Foundation "Structure and Sequence Variability Evaluated with a Computer-Vision Method" (#91-00219) 1992-1995 (with R. Nussinov)

EEO Officers Recognition Award, 1993

Grant from NIH Intramural Targeted Anti-Viral AIDS Program for "Improving Peptide Inhibitors for Receptor Targets", 1994-5, 1995-6

NIH Merit Award, 1995 *"in recognition of research contributions on protein and nucleic acid structures leading to deeper comprehension of conformations and biological functions"*

Grant, United States-Israel Binational Science Foundation "Probing Immunoglobulin Polyreactivity via Highly Efficient Docking, Fold Recognition and Kinetics" 1997-2000 (with R. Nussinov and H. Wolfson)

Grant, NATO Collaborative Research Grants Programme, 1996-1997 (with I. Bahar)

Fellow, The Institute for Advanced Studies, Hebrew University, Jerusalem, 1998-1999

Grant, "Deriving Structures for Lead Drug Discovery from Cell-Line Screens", DAMD17-98-1-8323, US Army Breast Cancer 1998-2001

Fellow, AAAS, 1999- Pres.

NIH-NSF Grant - BBSI: Summer Institute in Bioinformatics and Computational Biology (2002-2006) \$645,000

NIH Grant - Discovering Protein Sequence Structure Function Relationships (2003-2007) \$1,022,000

NIH Grant - Coarse-Grained Models of Protein (2004-2008) \$1,168,000

Sun Microsystems - Academic Equipment Grant (2004) \$86,880

NSF Grant - CNS MRI: Acquisition of a 512-node BlueGene/L Supercomputer for Large-Scale Applications in Genomics and Systems Biology (2005-2008) \$645,000

NIH - Modeling Ribosomal Control, Function and Assembly (2007-2011) \$1,060,380

NIH-NSF Grant - BBSI: Summer Institute in Bioinformatics and Computational Biology (2006-2008) \$499,999

10th most cited paper in the journal *Macromolecules*
http://pubs.acs.org/journals/mamobx/promo/40th/most_cited.html

ISU - Center for Integrated Animal Genomics - Comparative Genomics to Improve Livestock Gene Annotations (2007-2009) \$100,000

In top 5% of NIH intramurally supported researchers, 2008

Iowa State University Award for Excellence in Research, Iowa State University

Fellow, Biophysical Society

Teaching

Molecular Biophysics
 Structural Genomics
 Computational Biology

	Systems Biology
Research Fields	Biophysics Computational Biology Bioinformatics
Research Topics	Bioinformatics Computational Biology Structural Biology Molecular Computation Molecular Modeling Multi-scale Modeling Biomolecular Motions for Functions Protein Design to Control Function Biological Imaging Cell Simulations Systems Biology
Interests	Elucidation of the molecular details of biochemical and biophysical processes through the study of macromolecular conformations Computer modeling and simulations Development of coarse-grained structural principles Application of advanced computing to molecular calculations Protein and Cell Engineering and drug design Development of a combined experimental and theoretical methods to elucidate structures of proteins and nucleic acids Computer simulations of protein and RNA folding. Conformation enumeration of all chain tracings in restricted space of a given shape Effects of external conditions, including solvent and temperature, on the relative stabilities of macromolecular conformations Molecular interactions, recognition and specificity Nucleic acid conformational properties and their relationship to function, recombination and regulation Utilizing sequence similarities in conformational calculations Conformational transitions between ordered and disordered states, and between various ordered states Molecular visualization Dynamics of complex molecular assemblages, with the goal of constructing models of cellular processes such as mitosis Understanding protein sequence through structure Gene annotation through structural modeling Genome comparisons Bioinformatics methods Systems Biology
Scientific	Methods for averaging over conformations of flexible macromolecules

Accomplishments

Dynamic programming to choose optimum combination of protein secondary structures

Matrix methods for calculating electro-optic properties

Equilibrium pathway model for protein folding

Coarse graining of structures

Residue-residue interaction energies for proteins

Demonstration of weaker base pairings within promoter sequences

Large conformational fluctuations for different DNA sequences

Solvation model including structural water bridges

Calculation of sequence dependence of DNA double helix preferences for forms A or B

Generating and counting large numbers of diverse chain tracings for proteins and nucleic acids

Demonstration that intra-molecular interactions and solvation effects favor observed sequence dependences of DNA double helix groove variabilities

Derivation of amino acid substitution matrix from crystal structures

Treating RNA folding in three dimensions by generating chain tracings on lattice points

Treating peptide binding to surfaces of other macromolecules by generating peptide conformations on neighboring lattice sites

Modeling the bending of nucleic acid double helices around proteins

Calculations of favorable conformations of peptides and agreeing with NMR results

Description of TATA sequence box as a "swivel joint"

Identifying specific interacting pairs in a protein to effect conformational changes

Discovery of unique base triplets, with implications for recombination and replication

Discovery of high regularity of coordination geometry of protein ligands around cations

Established correlations between fluctuations in coarse-grained proteins and X-ray temperature factors and hydrogen exchange protection

Development of regular lattice from observed packing in protein crystals

Elastic networks and normal mode analyses to identify functional motions of coarse-grained proteins

Development of methods to calculate large scale motions in proteins

Establishing a connection between largest scale motions in Reverse Transcriptase and the nucleic acid processing steps

Identifying "wobble" motions in tubulin, related to its behavior

Identifying critical cavity surface changes arising from GroEL/GroES motions

Identifying critical motions of the ribosome and relating them to translocation

Networks as unifying models in biology
 Systems biology applications of networks
 Comprehending the highly coordinated motions of the ribosome

Meetings Organized

1990 – Organizer of Workshop in NIH Research Festival on Nucleic Acid-Protein Interactions
 1990 – Co-organizer with H. Scheraga of Cold Spring Harbor Conference on Computational Aspects of Protein Folding
 1992 – Co-organizer of NSF Molecular Dynamics Conference (Puerto Rico)
 1992 – Co-organizer of Workshop for NIH Research Festival on Structure Prediction with S. Bryant
 1992 – Co-organizer of Nucleic Acid Conference with V. Sasiesekharan, N. Leonard (Fogarty Scholars-in-Residence) and H. T. Miles
 1993 – Program Committee, Biophysical Society National Meeting
 1993 – Program Chair, NIH Inter-Institute Structural Biology Group
 1994 – Co-organizer of Cold Spring Harbor Meeting - Protein Folding and Design
 1994 – Co-organizer of Conference, "Frontiers in Biological Physics", La Jolla International School of Physics, The Institute for Advanced Physics Studies
 1999 – Organizing Committee, Eleventh Conversation in Biomolecular Stereodynamics
 2001 – Organizing Committee, 12th Conversation in Biomolecular Stereodynamics
 2003 - Iowa Bioinformatics Workshop
 2003 - Organizing Committee, 13th Conversation in Biomolecular Stereodynamics
 2004 - Iowa Bioinformatics Workshop
 2005 - Organizing Committee, 14th Conversation in Biomolecular Stereodynamics
 2005 - Iowa Bioinformatics Workshop
 2005 - Integration of Structural and Functional Genomic, ISU
 2006 - Steenbock Symposium on Dynamics of Proteins and Macromolecular Assemblies, Madison, WI

Theses

1987 – Regine Bohacek - Chemistry Department, Rutgers University
 1991 – David Bisant - Genetics Program, George Washington University
 2000–2001 – Isabelle Soury-Lavergne - Ecole Normal, Paris
 2002 – Committee of Sangyoon Lee - Johns Hopkins University, School of Engineering
 2004 – Moon-ki Kim - Johns Hopkins University, School of Engineering
 2005 - Haitao Cheng -M.S., Computer Science, ISU
 2006 - Peter Vedell - Ph.D., Mathematics and Bioinformatics and Computational Biology, ISU
 2007 - Myron Peto – Ph.D., Bioinformatics and Computational Biology, ISU
 2007 – Lei Yang – Ph.D., Bioinformatics and Computational Biology, ISU
 2008 – Aimin Yan – Ph.D., Bioinformatics and Computational Biology, ISU
 2008 – Yaping Feng – Ph.D., Biochemistry, Biophysics and Molecular Biology, ISU

Presentations and
Invitations - last 10
years

2009 – Haitao Cheng – Ph.D., Bioinformatics and Computational Biology, ISU

1998 – Invited Speaker, Biophysical Society, Kansas City, Symposium, Bioinformatics: Computer-Based Predictions of Protein Structure and Binding

1998 – Invitation to speak, “Protein Structure, Stability, and Folding. Fundamental and Medical Aspects”, Moscow

1998 – Invited Speaker, Symposium for New Center for Structural Biology, Tel Aviv University

1998 – Invited Speaker, Washington University, St. Louis

1998 – Invited Speaker, Weizmann Institute, Rehovot, Israel

1998 – Invited Speaker, Structural Biology Seminar, University of California, Berkeley

1999 – Plenary Lecturer – Conversation on Biomolecular Structure and Dynamics, Albany, NY

1999 – Invited Speaker, Proteins Gordon Conference, Holderness College, NH

1999 – Invited Speaker, University of California, San Francisco

1999 – Invited Speaker, Second Congress of Biophysicists of Russia, Moscow

1999 – Invited Speaker, Russian Biophysics Congress, Ptitsyn Memorial Symposium, Pushchino, Russia

1999 – Invited Speaker, Department of Chemistry, Pennsylvania State University

1999 – Invited Speaker, Department of Biological Chemistry, State University of New York, Stony Brook

2000 – Invited Speaker, MPSA 2000, Methods of Protein Structure Analysis, Charlottesville, VA

2000 – Invited Speaker, Danforth Plant Science Center and Washington University, St. Louis

2001 – Chair, Conversation on Biomolecular Structure and Dynamics, Albany, NY

2001 – Invited Speaker, “Protein folding, structure and design”, International Center for Theoretical Physics, Trieste, Italy

2001 – Invited Speaker, Department of Biochemistry, Biophysics and Molecular Biology, Iowa State University

2001 – Invited Speaker, Laboratory of Chemical Physics, NIDDK, NIH

2001 – Invited Speaker, Department of Biochemistry, Texas A&M University

2001 – Invited Speaker, Department of Biology, Georgia Tech

2001 – Invited Speaker, Department of Chemistry, University of Maryland

2001 – Invited Speaker, SUNY Buffalo School of Medicine

2001 – Invited Speaker, University of Colorado Health Sciences Center

2001 – Invited Speaker, Workshop, “Proteins as Machines”, College Park, MD

2001 – Invited Speaker, NEC America

2001 – Invited Speaker, Center for Studies in Physics and Biology, Rockefeller University

2001 – Invited Speaker, Center for Computational Biology & Bioinformatics, School of Medicine, University of Pittsburgh

2002 – Invited Speaker, Laboratory of Molecular Biology, National Cancer Institute

2002 – Invited Speaker, School of Engineering, Johns Hopkins University

2002 – Plenary Speaker, Joint Conference on Information Sciences, Durham, NC

2002 – Invited Speaker, “Proteomes: Structures, Changes, Interactions and Functions”, Ames, Iowa

2002 - Invited Speaker - Polymer Division, American Chemical Society

2003 - Invited Speaker - Chemistry Department, Iowa State University

2003 - Invited Speaker - Animal Breeding Group -Department of Animal Science, Iowa State University

2003 - Seventh Johns Hopkins Folding Meeting

2003 - Invited Speaker, Physics Department, Iowa State University

2003 - Invited Speaker - “Frontiers of Bioinformatics” Symposium, University of Buffalo, NY

2003 - Invited Speaker - “ Modeling of Protein Interactions in Genomes”, SUNY, Stony Brook, NY

2004 - Invited Speaker - Polymer Symposium, American Chemical Society, New York

2003 - Invited Speaker, Chemical Engineering Department, Iowa State University

2003 - Invited Speakers, Physics Department, Iowa State University

- 2004 - Invited Speaker, Center for Computational Biology, Washington University
- 2004 - Invited Speaker, Biomedicine Lecture Series, Des Moines University
- 2004 - Invited Speaker - "Frontiers in Chemistry", Case Western Reserve University
- 2004 - Invited Speaker - "Interplay between Computer Modeling and Experiments on Complex Biological Systems", American Chemical Society, Anaheim
- 2004 - Invited Speaker - Department of Biochemistry, Georgetown University Medical School
- 2005 - Invited Speaker - Center for Bioinformatics and Computational Biology, University of Iowa State University
- 2005 - Invited Speaker - Midwest Computational Structural Biology Workshop
- 2005 - Invited Speaker - International Center for Theoretical Physics, Trieste, Italy
- 2005 - Invited Speaker - Center for Bioinformatics and Computational Biology, College of Engineering, University of Iowa
- 2005 - Invited Speaker - Modeling of Protein Interactions in Genomes, Lawrence, KS
- 2005 - Invited Speaker - International Meeting on Relaxations in Complex Systems, Lille, France
- 2005 - Invited Speaker - Computational Biology Symposium - National Cancer Institute, Frederick MD
- 2005 - Invited Speaker - Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling: Bridging the Gap, Symposium, American Chemical Society, Washington, DC
- 2005 - Invited Speaker - Multiscale Workshop, Snowbird, UT
- 2005 - Invited Speaker - Department of Electrical and Computer Engineering, ISU
- 2005 - Invited Speaker - NIGMS, NIH, Bethesda
- 2006 - Invited Speaker - Biophysical Society, Workshop on Coarse-Grained Methods for Biomolecular Structure and Dynamics, Salt Lake City
- 2006 - Invited Speaker - Department of Chemistry, University of Oregon, Eugene
- 2006 - Invited Speaker - Workshop on Rigidity, Flexibility, and Motion in Biomolecules, Tempe, AZ
- 2006 - Invited Speaker - Workshop on Nanomechanics of Biomolecules,

Ascona, ETH Conference, Switzerland

2007 - Nebraska Research and Innovation Conference

2007 - 10th International Congress on Amino Acids and Proteins, Kallithea, Chalkidiki, Greece

2007 - Symposium on Structural Determination, Refinement and Modeling of Large Biomolecular Complexes (ACS Meeting, Boston)

2007 - Centenary Workshop on Multiscale Modeling in Biomolecular Systems, Imperial College, London

2007 - Indo-US Workshop on Spatial Kinematics and Protein Conformation, Bangalore

2008 - Protein Folding Symposium, Institute for Mathematics and Its Applications, University of Minnesota

2008 - Symposium - Multiscale Methods in Biophysics, American Chemical Society, New Orleans

2008 - Characterizing the landscape: from biomolecules to cellular networks, Telluride

2008 - Protein Structure & Mechanics, Shanghai

2008 - Forefronts of Genomics, University of California, Davis

2008 - Multiscale Modeling in Soft and Biological Matter, University of Minnesota

2009 - Structural Biology Department, Hauptman-Woodward Medical Research Institute and Roswell Park Cancer Center

2009 - Multiscale Soft Matter, Groningen

2009 - CECAM - Coarse-Graining Biological Systems: Towards Large-Scale Interactions and Assembly, Lausanne

2009 - Protein Function and Dynamics, Beijing

2009 - Algorithms in Macromolecular Modeling Conference, University of Texas, Austin

Reviews

Recent Review Panels:

NIH F04B March 2003, November 2003, March 2004 (Biophysics, Biochemistry Fellowships Panel)

NIH Special "Roadmap" Study Section for National Centers, ZRG1 BST-C May 2004

NSF Science and Technology Center Site Visit Review Committee, June 2004

NIH Computational Biophysics Study Section, October 2004

Chair, NSF Frontiers in Physics Center and Large ITR Site Visit, December 2004

NIH Special Study Section, 2005

DOE Early Career Principal Investigator Program, 2006
 NSF Bioinformatics Postdoctoral Panel, 2006
 NIH Special Study Section ZRG1 BCMB-B, 2006
 Chair, NSF Frontiers in Physics Center and Large ITR Site Visit, 2006
 NIH Study Section ZRG1 BCMB-B Biological Chemistry and Macromolecular
 Biophysics 2007
 NSF Panel Physics Frontier Centers 2007, 2008
 NSF Bioinformatics Postdoctoral Panel, 2007, 2008, 2009
 NIH AED Review Panels 2007, 2008, 2009
 NSF TeraGrid Review 2009
 NIH Challenge Grant AED Reviews 2009
 NIH Musculoskeletal, Oral and Skin Sciences Review Group 2009

Journals: Journal of the American Chemical Society, Journal of Biological Chemistry, Biochimica et Biophysica Acta, Journal of Chemical Physics, Science, Nature, Proceedings of the National Academy of Science USA, Biophysical Chemistry, Journal of Molecular Biology, Macromolecules, Biochemistry, Journal of Polymer Science, Biopolymers, Journal of Biomolecular Structure and Dynamics, FASEB Journal, Chemical Physics, Protein Science, Journal of Mathematical Chemistry, Proteins, Journal of Computer-Aided Molecular Design, Europhysics Letters, Journal of Physical Chemistry, Nucleic Acids Research, Computational Polymer Science, Protein Engineering, Folding & Design, Physical Review, IBM Systems Journal, Bioinformatics, BMC Bioinformatics, and others

Student Selection, Faculty Tenure and Search Committees: Pioneer Fellowship Committee - Iowa State University, many NIH committees, Cornell Univ., Boston University, physics search - Iowa State University, Chief Information and Technology Officer search - Iowa State University, and many other academic promotion and tenure reviews (6 during November 2006)

Grant Reviews: Defense Threat Reduction Agency, NIH Special Study Sections including BST-C-R NIH Study Section - National Centers for Biomedical Computing (2004), BST-C Study Section Special Emphasis Panel on Cryo-electron microscopy (2004), NSF Site Visit Science and Technology Center (2004), F04 NIH Ruth L. Kirschtein National Research Service Application Study Section (2003, 2004), World Bank Panel on Biodiversity (2004), Nebraska Research Initiative (2004), Texas A&M Research Initiative, NSF Frontiers in Physics Review Panel, Genome Research Review Committee (NHGRI), The Wellcome Trust (Joint Infrastructure Fund, UK), NIH Biophysical and Chemical Sciences Review Group, NIH Special Study Sections, Plant Sciences Institute ISU, NSF, NIDA, NIH Program Project Special Study Section, NIH Special Emphasis Panel, NIH Fogarty Scholar-in-Residence Program, DOE, NSF Supercomputer Centers, Advanced Scientific Computing Laboratory - FCRDC, NSF Multidisciplinary Research Review Panel, Packard Foundation, Guggenheim Foundation, Petroleum Research Fund and International Science Foundation, NIH CIT Computational Science and Engineering Program Review and others

Research Management

Computational Molecular Biology Research Group Initiated
 Microarray Research Group Initiated
 Systems Biology Research Group Initiated
 Organized Seminar Series
 Organized Advisory Committees
 Organized Large Grant Applications

Present Funding

- NIH R01GM72014 (PI: Jernigan) Coarse Grained Proteins (2009-2014)
\$1,755,000
- NIH-NSF Joint EEC-0608769 (PI: Jernigan) BBSI Bioinformatics and
Computational Systems Biology Summer Institute at Iowa State (2006-
2009) \$499,999
- NIH R01GM073095 (PI: Jernigan) Modeling Ribosomal Control, Function and
Assembly, (2006-2010) \$1,060,380
- NIH R01GM081680 (PI: Kloczkowski) High-Accuracy Protein Models Derived
from Lower Resolution Data (2007-2010) \$750,000
- DOE DE-FG02-08ER64579 Nanoimaging to Prevent and Treat
Alzheimer's and Parkinson's Diseases Sub-Contract with
University of Nebraska Medical Center (PI: Lyubchenko, Univ.
Nebraska) (2008-2010) \$100,000
- ISU - Center for Integrated Animal Genomics (PI: Jernigan) Comparative
Genomics to Improve Livestock Gene Annotations (2007-2009)
\$100,000