

Robert L. Jernigan

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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, NIH
- 1992 – 2002* Chief, Section on Molecular Structure, NIH
- 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
- 2012 – Pres.* Affiliate Professor, Department of Physics, Iowa State University
- 2013 – Pres.* Affiliate Professor, Department of Computer Science, 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 – 2007 Publications Committee, Biophysical Society overseeing
Biophysical Journal
- 2003 – 2007 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 Committee, Minnesota Supercomputing
Institute, Univ. Minn.
- 2005 – 2010 External Advisory Committee, Tuskegee University (NSF
HBCU-HP)
- 2004 – *Pres.* Departmental Promotion and Tenure Committee
- 2007 – *Pres.* Research Computing Council (ISU)
- 2008 – Program Committee for Intelligent Systems for Molecular
Biology
- 2008- 2011 Program Committee for European Conference on
Computational Biology
- 2009 – 2011 Program Committee International Society for
Computational Biology
- 2010 – *Pres.* ISU Steering Committee for Interdisciplinary Applied
Scientific Computation
- 2010 – *Pres.* Member, Advisory Board, New Mexico State University,
CREST Center for Bioinformatics and Computational Biology
- 2010 – *Pres.* – Member, Advisory Committee on Bioinformatics,
George Washington University
- 2010, 2011 – Chair, National Academy, Molecular Dynamics ANTON
Award Committee
- 2011 – ISU Steering Committee on High Performance Computing
- 2014 – Department of Mathematics, Iowa State University, Search
Committee for Mathematical Biology
- Presently* – Program of Study Committees – 24 graduate students

Memberships

Biophysical Society
 Protein Society
 American Society for Biochemistry and Molecular Biology
 RNA Society
 International Society for Computational Biology

Current editorial boards

Biochemistry
 Bioinformatics and Biological Insights
 Journal of Data Mining in Genomics & Proteomics
 Review Editor, Frontiers in Molecular Biosciences

Awards

NIH Special Achievement Cash Award, 1982
 EEO Officers Recognition Award, 1993
 NIH Merit Award *"in recognition of research contributions on protein and nucleic acid structures leading to deeper comprehension of conformations and biological functions,"* 1995
 Fellow, The Institute for Advanced Studies, Hebrew University, Jerusalem, 1998-1999
 Fellow, AAAS, 1999
 In top 5% of NIH intramural supported researchers, 2008
 Iowa State University Award for Excellence in Research, 2008
 Fellow, Biophysical Society, 2009
 Gamma Sigma Delta Faculty Honor Society, 2011
 NIH Service Award for frequent grant reviews, permitting continuous grant submissions, at any time, regardless of deadlines, 2010-2014

Past Grants

NIH Intramural Targeted Anti-Viral AIDS Program
 Calculations of Preferred Ligands of the HIV-1 Protease Surface, 1990-2
 NIH Intramural Targeted Anti-Viral AIDS Program
 Enzyme Binding Sites for Peptides, 1992-4
 United States-Israel Binational Science Foundation
 Structure and Sequence Variability Evaluated with a Computer-Vision Method (#91-00219) 1992-5 (with R. Nussinov)
 NIH Intramural Targeted Anti-Viral AIDS Program for
 Improving Peptide Inhibitors for Receptor Targets, 1994-6
 United States-Israel Binational Science Foundation - Probing Immunoglobulin Polyreactivity via Highly Efficient Docking, Fold Recognition and Kinetics 1997-2000 (with R. Nussinov and H. Woolfson)
 NATO Collaborative Research Grants Programme, 1996-7
 (with I. Bahar)
 US Army Breast Cancer - Deriving Structures for Lead Drug Discovery from Cell-Line Screens, 1998-2001
 NIH-NSF BBSI: Summer Institute in Bioinformatics and Computational Biology, 2002-6
 NIH R21 - Discovering Protein Sequence Structure Function Relationships, 2003-7
 Sun Microsystems - Academic Equipment, 2004
 NSF - CNS MRI - Acquisition of a 512-node BlueGene/L Supercomputer for Large-Scale Applications in Genomics and Systems Biology, 2005-8
 ISU - Center for Integrated Animal Genomics - Comparative

Genomics to Improve Livestock Gene Annotations, 2007-9
NIH-NSF Grant - BBSI: Summer Institute in Bioinformatics and
Computational Systems Biology, 2006-10
DOE - Nanoimaging to Prevent and Treat Alzheimer's Disease, 2008-10
NIH R01 – High-Accuracy Protein Models Derived from Lower
Resolution Data
NIH R01 Coarse Grained Proteins (2009-2014) \$1,755,000
NIH R01 Modeling Ribosomal Control, Function and Assembly, (2006-2013)
\$1,060,380
USDA Hatch Act Salary Support – Project – Structural and Functional Genomic:
(2006-present)

Research Fields

Biophysics
Computational Chemistry
Computational Biology
Bioinformatics
Structural Biology
Systems Biology
Datamining
Simulation Science

Research Topics

Molecular Computations and Simulations
Molecular Modeling
Drug Selection
Datamining
Multi-scale Modeling
Biomolecular Motions for Functions
Protein Design to Control Function
Molecular Mechanisms
Cell Imaging
Cell Simulations
Building Molecular Machines

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
Protein and Cell Engineering
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 within 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 directly 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
 Using protein interaction data to construct molecular machines

Scientific Accomplishments

Methods for averaging over conformations of flexible macromolecules
 Dynamic programming to choose optimum combination of protein secondary structures
 Matrix methods for calculating physical 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
 Sequence-dependent conformational fluctuations for different DNA sequences
 Calculation of sequence dependence of DNA double helix preferences
 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
 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 lattices 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 very large structures
 Establishing a mechanistic connection between large scale motions in Reverse Transcriptase and the nucleic acid processing steps
 Identifying “wobble” motions in tubulin, related to its behavior
 Identifying internal cavity changes in GroEL/GroES that assist protein unfolding
 Identifying critical motions of the ribosome and relating them to translocation
 Comprehending the highly coordinated motions of the ribosome in its mechanism
 Networks as unifying models in biology
 Development of methods to extract dynamics from sets of crystal structures
 Methods to treat explosive exothermic reactions, such as ATP hydrolysis

Meetings Organized

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
 2009 – Systems Biology: Integrative, Comparative and Multi-Scale Modeling at

Iowa State University

- 2009 – Iowa State University Bioinformatics Research Fair
- 2010 – RNA in Motion, ISU
- 2010 – Telluride Science Research Center - Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules
- 2011 – Zing Conference - Protein and RNA Structure Prediction Conference, Mexico
- 2012 – Telluride Science Research Center - Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules

- 2013 – Telluride Science Research Center – Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules
- 2013 – Zing Conference - Protein and RNA Structure Prediction Conference, Mexico
- 2014 – Telluride Science Research Center – Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules
- 2014 – Zing Conference on Protein Folding, Dominican Republic

Theses

- 1987 – Regine Bohacek - Chemistry Department, Rutgers University
- 1991 – David Bisant - Genetics Program, George Washington University
- 2001 – Isabelle Soury-Lavergne - Ecole Normale, Paris
- 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
- 2009 – Haitao Cheng – Ph.D., Bioinformatics and Computational Biology, ISU
- 2011 – Saraswathi Sundararajan – Ph.D., Bioinformatics and Computational Biology, ISU
- 2011 – Sumudu Leelananda – Ph.D., Bioinformatics and Computational Biology, ISU
- 2011 – Michael Zimmermann – Ph.D., Bioinformatics and Computational Biology, ISU
- 2013 – Aatur Katebi – Ph.D., Bioinformatics and Computational Biology, ISU
- 2013 – Scott Boyken – Ph.D., Bioinformatics and Computational Biology, ISU
- 2013 – Yuanyuan Huang – Ph.D., Bioinformatics and Computational Biology, ISU

Presentations and Invitations

- 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 Speaker, 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

- 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 – Invited Speaker - Nebraska Research and Innovation Conference
- 2007 – Invited Speaker - International Congress on Amino Acids and Proteins, Kallithea, Chalkidiki, Greece
- 2007 – Invited Speaker - Symposium on Structural Determination, Refinement and Modeling of Large Biomolecular Complexes (ACS Meeting, Boston)
- 2007 – Invited Speaker - Centenary Workshop on Multiscale Modeling in Biomolecular Systems, Imperial College, London

- 2007 – Invited Speaker - Indo-US Workshop on Spatial Kinematics and Protein Conformation, Bangalore
- 2008 – Invited Speaker - Protein Folding Symposium, Institute for Mathematics and Its Applications, University of Minnesota
- 2008 – Invited Speaker - Symposium - Multiscale Methods in Biophysics, American Chemical Society, New Orleans
- 2008 – Invited Speaker - Characterizing the landscape: from biomolecules to cellular networks, Telluride
- 2008 – Invited Speaker - Protein Structure & Mechanics, Shanghai
- 2008 – Forefronts of Genomics, University of California, Davis
- 2008 – Invited Speaker - Multiscale Modeling in Soft and Biological Matter, University of Minnesota
- 2009 – Invited Speaker - Structural Biology Department, Hauptman Woodward Medical Research Institute and Roswell Park Cancer Center
- 2009 – Invited Speaker - Conference on Multiscale Soft Matter, Groningen
- 2009 – Invited Speaker - CECAM - Coarse-Graining Biological Systems: Towards Large-Scale Interactions and Assembly, Lausanne
- 2009 – Invited Speaker - BioMAP, Rutgers University
- 2009 – Invited Speaker - Laufer Center for Computational Biology and Genome Sciences, Stony Brook University
- 2009 – Invited Speaker - Biological Sciences, Columbia University
- 2009 – Invited Speaker - Algorithms in Macromolecular Modeling Conference, University of Texas, Austin
- 2010 – Invited Speaker - Distinguished Speaker, University of Pittsburgh
- 2010 – Invited Speaker - Department of Chemistry, Pennsylvania State University
- 2010 – Invited Speaker - Physics Department, Iowa State University
- 2010 – Invited Speaker - Department of Chemistry, University of Cincinnati
- 2010 – Invited Speaker - Department of Chemistry and Physics, University of Missouri
- 2010 – Invited Speaker - NIH Workshop on Enabling Technologies for Structure & Function
- 2010 – Invited Speaker - NIH-NSF Frontiers in Mathematical Biology, University of Maryland
- 2010 – Invited Speaker - RNA in Motion Conference, Iowa State University
- 2010 – Invited Speaker - Modeling of Protein Interactions Meeting, University of Kansas
- 2010 – Invited Speaker - Genetics, Development and Cell Biology Department, Iowa State University
- 2011 – Invited Speaker - Biochemistry Colloquium, University of Wisconsin
- 2011 – Invited Speaker - International Conference on Mathematical Biology, Bangalore
- 2011 – Invited Speaker - Conference on Analysis and Simulation of

- Biomolecular Structures, Bangalore
- 2011 – Invited Speaker – Telluride Science Research Center – Modeling Biomolecular Structures, Interactions and Functions
- 2011 – American Chemical Society Symposium Denver - Predicting and Disrupting Protein Interactions
- 2011 – Symposium Honoring Harold Scheraga on his 90th Birthday – Cornell University
- 2011 – Physics Department Colloquium – University of Buffalo
- 2011 – Invited Speaker and Organizer - Zing Conference – Protein and RNA Structure Predictions, Mexico
- 2012 – Invited Speaker – Telluride Science Research Center - Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules
- 2012 – Invited Speaker – Department of Biology, University of North Texas
- 2012 – Invited Speaker – Arkansas Bioscience Institute, Arkansas State University
- 2012 – Invited Speaker – Center for Biological Physics, Arizona State University
- 2012 – Invited Speaker – Modeling of Protein Interactions Conference, University of Kansas
- 2012 – Invited Speaker – Morgridge Institute, University of Wisconsin
- 2012 – Invited Speaker – Zing Conference on Mathematical Medicine
- 2013 – Invited Speaker – University of California, Irvine
- 2013 – Invited Speaker – Dynamics Conference, Durham University, UK
- 2013 – Invited Speaker, University of Arkansas, Protein Bioinformatics
- 2013 – Invited Speaker, Biology and Biochemistry Department, University of Houston
- 2013 – Invited Speaker, Modeling Biomolecular Structures, Interactions and Functions, Telluride
- 2013 – Invited Speaker, “Rise of the Machines” on Complex Molecular Systems , Telluride
- 2013 – Invited Speaker, Nationwide Children’s Hospital, Ohio State University
- 2013 – Invited Speaker, 18th Conversation on Biomolecular Structure and Dynamics, Albany
- 2013 – Invited Speaker, Symposium on Coarse-grained Structures, American Chemical Society National Meeting, Indianapolis
- 2013 – Invited Speaker, Zing Mathematical and Computational Medicine, Cancun
- 2014 – Invited Speaker, Challenges in RNA Structural Modeling and Design, Telluride
- 2014 – Invited Speaker, Modeling of Biomolecular Systems Dynamics, Allostery and Regulation: Bridging Experiments and Computations, Istanbul
- 2014 – Invited Speaker, Significance of Knotted Structures for Function of Proteins and Nucleic Acids, Warsaw
- 2014 – Invited Speaker, Department of Computational Medicine and Bioinformatics, University of Michigan Medical School
- 2014 – Invited Speaker, Raymond and Beverly Sackler Institute for Biological, Physical and Engineering Sciences, Yale University
- 2014 – Chair/Discussion Leader, Biopolymers Gordon Research Conference
- 2014 – Invited Speaker, Modeling of Protein Interactions, University of Kansas

Reviews

- NIH Special “Roadmap” Study Section for National Centers for Biomedical Computing, ZRG1 BST-C, 2004
- BST-C Study Section Special Emphasis Panel on Cryo-electron microscopy,

2004

NSF Science and Technology Center Site Visit, 2004
NIH Ruth L. Kirschstein National Research Service Application Study Section, 2004
NIH Computational Biophysics Study Section, 2004
Chair, NSF Frontiers in Physics Center and Large ITR Site Visit, 2004
World Bank Panel on Biodiversity, 2004
Nebraska Research Initiative, 2004
Texas A&M Research Initiative, 2005
NIH Special Study Section, 2005
Genome Research Review Committee (NHGRI), 2005
The Wellcome Trust (Joint Infrastructure Fund, UK), 2005
NIH Biophysical and Chemical Sciences Review Group, 2005
NIH Program Project 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 Panel, 2009
NIH Challenge Grant AED Reviews, 2009
NIH Musculoskeletal, Oral and Skin Sciences Review Group, 2009
NIH Special Emphasis Panel BCMB-B, 2009
Defense Threat Reduction Agency, 2009, 2010
Chair, NAS Review Panel on Supercomputing, ANTON, 2010
NIH Special Emphasis Panel on New Biomedical Frontiers at the Interface of Life and Physical Sciences, 2010
NIH Molecular Structure and Function D, 2011
NSF Site Visit Physics Frontier Center, 2011
Chair, NAS Review Panel on Supercomputing, ANTON, 2011
NIH IAR Study Section, 2011
NIBIB Training Grant Study Section, 2011
NIH-NSF Study Section on Interface between Life and Physical Sciences, 2011
NIH Intramural Review Team – NCI, Laboratory of Molecular Biology, 2011
Institut National du Cancer, mesothelioma review, France, 2011, 2012
NIH Single Molecule Study Section Spring 2012
NIH MSFD Study Section 2012, Spring and Fall
NIH Training Grant Study Section, Fall 2012
Institut National du Cancer, France, grant reviews, 2011, 2012
NSF Science and Technology Center Site Visit, Buffalo, Fall 2012
NIH 2013/05 ZRG1 MOSS-C (56) R RFA RM12-016: NIH Director's New Innovator Award Study Section 2013
NIH Mid-Point Evaluation of Protein Structure Initiative: Biology Program, 2013
NIH 2013/05 ZRG1 BCMB-B (02) M Biological Chemistry and Macromolecular Biophysics Study Section, 2013
Chair, NSF Site Visit, Center for Theoretical Biological Physics – Physics Frontier Center, Rice University, 2013
AAAS Review Panel, South Dakota, 2013
NSF Panel - Physics Frontier Center Pre-Applications, 2013
NSF Physics Frontier Center Site Visit, 2013

NIH Director's New Innovator Reviews, 2014
NIH Big Data to Knowledge Study Section 2014
NIH Training Grants – NIBIB 2014

Other Grant Reviews: NIH Fogarty Scholar-in-Residence Program, DOE, NSF Supercomputer Centers, Review of NRC Review, Advanced Scientific Computing Laboratory - FCRDC, NSF Multidisciplinary Research Review Panel, Packard Foundation, Guggenheim Foundation, Petroleum Research Fund, International Science Foundation, Human Frontiers, NIH CIT Computational Science and Engineering Program Review and many others

Journals: PLoS One, PLoS Computational Biology, BMC Bioinformatics, Bioinformatics, Biophysical Journal, Physical Review Letters, Journal of Medicinal Chemistry, Structure, 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, Science, Nature, IBM Systems Journal, Bioinformatics, and many 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 numerous academic promotion and tenure reviews

Center Management

Organized Seminar Series with Many Outside Speakers
Computational Molecular Biology Research Group
Discussion Groups Organized:
 Systems Biology Research Group
 NextGen Sequencing Research Group
 ENCODE Discussion Group
Biological Imaging Research Group
Organized Grant Applications
Mentored Young Faculty – helped Assistant Professor (Computer Science) obtain NSF Career Award upon first application
Provided cost-sharing to strengthen grant applications
Supervised bioinformatics assistance team
Assisted in development of training grant applications
Assisted users with hardware and software
Annual research fair
Retreat
Provided support for graduate students and postdoctoral fellows
Provided support for travel
Supported ISU symposia
Supported faculty web sites
Supported Summer Institute in Computational and Systems Biology
Provided support for computer hardware and software
Provided computer access to Center Clusters
Center servers for distributing software and providing access to software

Nominated and organized support for national awards for faculty and students
Developed plans for Center's continued growth with > 30% annual increases
during 2006-2012

Present Funding

NSF MCB-1021785 (PI: Jernigan) Structural Interpretation of Protein Interactomes (2010-2014)
ISU Plant Science Support for Baker Center – salaries and computers
USDA Hatch Act IAHEES project (PI: Jernigan) Structural and Functional Genomics (2011-present salary support)
ISU PSI Seed Grant (PI: Bassham) Imaging of Growing Plants and Computational Modeling of Plant Growth and Development
ISU Presidential Initiative for Interdisciplinary Research RNA Therapeutic Targets in Infectious Disease 2013-2014
ISU Presidential Initiative for Interdisciplinary Research Award Integrated, Interdisciplinary Vaccine Research Against Antigenically Diverse Viruses
ISU LAS Signature Initiative Award Engineering plant proteins to treat stroke and myocardial infarction (PI: Mark Hargrove)
NSF TeraGrid and Xsede (NSF) Awards of Computing Time 2011-2013

Funding under Review or To Be Submitted Soon

NSF - Development of a New Generation of Free Energies for Protein Model Evaluations, with Andrzej Kloczkowski (Research Institute at Nationwide Children's Hospital)

NIH - Computational Design of Influenza Hemagglutinin Inhibitors, with Andrzej Kloczkowski (Research Institute at Nationwide Children's Hospital), Lynne Regan (Yale University), Corey O'Hern (Yale University), Jianpeng Ma (Baylor College of Medicine), Qinghua Wang (Baylor College of Medicine)

NIH – Visualization of Rotational Dynamics of Cellular Membrane Processes

NSF – Collaborative Research: Protein Prediction Using Crystal Space Group Symmetry, with Andrzej Kloczkowski (Research Institute at Nationwide Children's Hospital), Gregory Chirikjian (Mechanical Engineering, Johns Hopkins University)

NIH renewal – Comprehending the Mechanism of the Ribosome

NIH renewal – Coarse-Grained Models of Proteins and RNA with Andrzej Kloczkowski (Research Institute at Nationwide Children's Hospital)

NSF – RNA-Protein Interactions, with Drena Dobbs, Vasant Honavar

NSF– Directed Driving Forces from ATP and GTP Hydrolysis

NSF – Visualizing the Endoplasmic Reticulum and Its Mechanisms, with Diane Bassham and Julie Dickerson

NSF – NRT DESE – Molecular BioSystems (MBS): Data-Enabled Protein and RNA Engineering, with Basil Nikolau, Drena Dobbs, Adah Leshem, and Surya Mallapragada

NIH – Understanding Molecular Details of Antibody Maturation, with Richard Honzatko

FDA Improved Computational Analyses of Drug Assays, with Fadi Towfic (Immuneering) and Teva Pharmaceutical Industries

NIH – Extracting the Most from High Throughput Data

Recent Student
Outcomes

Ataur Katebi (Ph.D. 2013) postdoc, NIH, Lab of Molecular Biology, NCI, Bethesda

Scott Boyken (Ph.D. 2013) postdoc, David Baker lab, University of Washington, Seattle

Saras Saraswathi (Ph.D. 2011) postdoc Nationwide Children's Hospital, Batelle Center for Mathematical Medicine, Columbus, OH

Sumudu Leelananda (Ph.D. 2011) postdoc, Albert Einstein School of Medicine, NYC in Andras Fiser lab

Michael Zimmermann (Ph.D. 2011) postdoc, Mayo Clinic, Rochester, MN

Andrzej Kloczkowski (postdoc until 2010) now Professor, Ohio State University School of Medicine

Yaping Feng (Ph.D. 2009) Scientist, Waksman Genomics Center, Rutgers University, NJ

Since arriving at Iowa State University in 2002, he has trained in addition another 4 postdocs and 3 graduate students who all have scientific careers. One is a research scientist at USDA, one is at Dana-Farber Cancer Institute in Boston, one at Dupont Pioneer in Johnston, IA, one at Oregon Health Sciences University, one is an Associate Professor in Computer Science at Iowa State University. Prior to being at Iowa State University, he trained many postdocs who now have research careers, and one of the most outstanding is Ivet Bahar who is the founder of the Department of Computational and Systems Biology at the University of Pittsburgh School of Medicine.