Tod D. Romo

Univ. of Rochester Medical Center
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RESEARCH EXPERIENCE & EDUCATION

Staff Scientist, Biochemistry & Biophysics **2014 - Current**

University of Rochester Medical School, Rochester, NY

- iOS/Swift applications
- Molecular dynamics simulations of synuclein core assembly and stability
- Long time-scale molecular dynamics simulations of lysozyme and modeling of terahertz spectra
- Long time-scale molecular dynamics simulations of antimicrobial lipopeptides in membranes
- Pattern recognition methods for molecular dynamics analysis
- Software development and support for structural analysis (LOOS)
- Internal automated results validation system for lab software
- Continuous integration support for lab software
- Support for script-based software for maintenance of long time-scale MD simulations
- Data and molecular visualization applications and methodology development
- Mentor and train graduate and undergraduate students

Postdoctoral Research Associate, Biochemistry & Biophysics **2008 - 2014**

University of Rochester Medical School, Rochester, NY

- Multi-scale simulations of G protein-coupled receptors in membranes
- Long time-scale molecular dynamics simulations of antimicrobial lipopeptides in membranes
- Development and analysis of elastic network models (part of LOOS)
- Methods for molecular dynamics convergence analysis
- Pattern recognition methods for molecular dynamics analysis
- Software design for structural analysis (LOOS)
- Developed script-based software for maintenance of long time-scale MD simulations
- Molecular visualization support and development
- Mentor and train graduate, undergraduate, and high school students

Research Scientist, Center for Structural Biology **2001 - 2006**

Institute for Biosciences and Technology / Texas A&M, Houston, TX

- Development and application of pattern recognition, optimization (including parallel programming), and sequence alignment algorithms for automated crystallographic model determination within TEXTAL™
- Integration of TEXTAL™ with PHENIX—the next generation of software for structural determination.
- Porting and deployment of TEXTAL™ to multiple architectures.
- Web services development and cryptographic licensing utilities for TEXTAL™.
- Coordinator for the Keck Center for Bioinformatics VR facility at the IBT in Houston, TX
- Coordinator for the Biochemistry and Biophysics VR facility at Texas A&M in College Station, TX
- Virtual reality interface design for directed crystallographic model building and structural analysis.
- Bioinformatics applications for targeting and cloning pipeline optimization for the Tuberculosis Structural Genomics Consortium.
- On-line database for tracking collaborative cloning pipeline progress
- Unix system administration and networking infrastructure support

Postdoctoral Research Associate **Fall, 1998 - Spring, 2001**

Rice University, Houston, TX

- Development of VR systems for the visualization of crystallographic data and protein structures for high throughput crystallography applications
- Development of immersive VR environments for teaching macromolecular biophysics
- Design and implementation of web-based tracking systems for crystallographic experimental data
- Bioinformatics and clone database mining

Doctor of Philosophy, Rice University, Houston, TX **1991 - 1998**

Adviser: George N. Phillips, Jr., PhD
Department: Biochemistry and Cell Biology
Thesis: Identification and Modeling of Protein Conformational Substates
Awards: W. M. Keck Center for Computational Biology Predoctoral Fellowship

Summer Research Fellowship **Summer, 1991**

Trinity University / Brooks AFB, San Antonio, TX

- Automated identification of foci in Mouse RAW Macrophages using light microscopy
- Supervising professor: Robert V. Blystone, PhD

Bachelor of Science, Trinity University, San Antonio, TX **Spring, 1991**

Department: Biology (BS)
Department: Mathematics (BS)
Advisor: Robert V. Blystone, PhD

Undergraduate Research **Fall, 1987 - Spring 1991**

Trinity University, San Antonio, TX

- Digital image processing for light and electron microscopy (Supervisor: Robert V. Blystone, PhD)
- Analysis of Perpendicular Arrays (Supervisor: Maurice Eggen, PhD)
- Microbiology and animal physiology lab assistant (Supervisor: Rex Moyer, PhD)
- Data analysis and digitization (Supervisor: Glenn Kroeger, PhD)

EDUCATION EXPERIENCE

Guest Lecturer

Fall, 2009 CHM 470 "Computational Chemistry" at University of Rochester, "The β_2-Adrenergic Receptor: Simulation and Analysis"
Spring, 2006 BIOS 533 "Computational Biology" at Rice University, "From Sequence to Journal Cover: Model Prediction & Visualization"
Spring, 1998 BIOS 590 "Special Topics" at Rice University, "Rendering and Animation for Molecular Visualization."
1993 Workshop on Digital Microscopy at the American Society for Cell Biology meeting in New Orleans, LA, including hands-on lab.
1992 Workshop on Digital Microscopy at the American Zoological Society meeting in Vancouver, BC, including hands-on lab.

Student Mentor/Supervisor

2009–2016 Mentoring and training graduate students (N. Leioatts, J. Horn, D. Lin, S. Sur, and L. Estrada)
2010 Mentored and trained high school student (K. Hu)
2008–2009 Mentored and trained undergraduate student (M. Jenkins)
2003–2004 Supervised Monterey Tech, MX, medical student summer projects at IBT, including use of the IBT VR facility for docking studies.

2002–2003 Supervised undergraduate (V. Reddy) in C++, VR, OpenGL, and concurrent programming in College Station developing iStitch, an interactive component of TEXTAL™.

1999–2001 Supervised undergraduates for basic programming and VR development skills, adapting the VMD package for use with x-ray data and modeling.

Facility Coordinator

2001–2006 Coordinator for the Keck Center for Bioinformatics VR facility at IBT and the VR Facility in Biochemistry and Biophysics at Texas A&M in College Station.

1998–2001 Coordinator for the VR Facility in Biochemistry & Biophysics at Rice University.

Computer Support/Lab Support/Teaching Assistant

1999 & 2000 BIOS 535 "Practical Crystallography" at Rice University

1997 Keck Center for Computational Biology sponsored K-12 outreach program with the Rice School using the Interplanetary Society's RedRover™ course.

1993 Physical Chemistry at Rice University

1992 Cell and Molecular Biology at Rice University

HONORS

- W. M. Keck Center for Computational Biology Predoctoral Fellowship
- Sigma Xi
- Beta, Beta, Beta Biology Honors Society
- National Merit Scholar

PUBLICATIONS

1. Leioatts, N., Romo, T. D., Danial, S. A. & Grossfield, A. Retinal Conformation Changes Rhodopsin's Dynamic Ensemble. Biophys J 109, 608–617 (2015).
2. Romo, T. D., Leioatts, N. & Grossfield, A. Lightweight object oriented structure analysis: tools for building tools to analyze molecular dynamics simulations. J. Comput. Chem. 35, 2305–2318 (2014).
3. Romo, T. D. & Grossfield, A. How fast is your camera? Timescales for molecular motion and their role in restraining molecular dynamics. Biophys J 106, 2549–2551 (2014).
4. Leioatts, N., Suresh, P., Romo, T. D. & Grossfield, A. Structure-based simulations reveal concerted dynamics of GPCR activation. Proteins 82, 2538–2551 (2014).
5. Romo, T. D. & Grossfield, A. Unknown Unknowns: the Challenge of Systematic and Statistical Error in Molecular Dynamics Simulations. Biophys J 106, 1553–1554 (2014).
6. Leioatts, N. et al. Retinal ligand mobility explains internal hydration and reconciles active rhodopsin structures. Biochemistry 53, 376–385 (2014).
7. Horn, J. N., Romo, T. D. & Grossfield, A. Simulating the mechanism of antimicrobial lipopeptides with all-atom molecular dynamics. Biochemistry 52, 5604–5610 (2013).
8. Leioatts, N., Romo, T. D. & Grossfield, A. Elastic Network Models are Robust to Variations in Formalism. J Chem Theory Comput 8, 2424–2434 (2012).
9. Horn, J. N., Sengillo, J. D., Lin, D., Romo, T. D. & Grossfield, A. Characterization of a potent antimicrobial lipopeptide via coarse-grained molecular dynamics. Biochim Biophys Acta 1818, 212–218 (2012).
10. Romo, T. D. & Grossfield, A. Block Covariance Overlap Method and Convergence in Molecular Dynamics Simulation. J Chem Theory Comput 7, 2464–2472 (2011).
11. Romo, T. D., Bradney, L. A., Greathouse, D. V. & Grossfield, A. Membrane binding of an acyl-lactoferricin B antimicrobial peptide from solid-state NMR experiments and molecular dynamics simulations. Biochim Biophys Acta 1808, 2019–2030 (2011).
12. Romo, T. D. & Grossfield, A. Validating and improving elastic network models with molecular dynamics simulations. Proteins 79, 23–34 (2011).
13. Hurst, D. P. et al. A lipid pathway for ligand binding is necessary for a cannabinoid G protein-coupled receptor. J Biol Chem 285, 17954–17964 (2010).
14. Romo, T. D., Grossfield, A. & Pitman, M. C. Concerted interconversion between ionic lock substates of the beta(2) adrenergic receptor revealed by microsecond timescale molecular dynamics. Biophys J 98, 76–84 (2010).

15. Romo, T. D. & Grossfield, A. LOOS: an extensible platform for the structural analysis of simulations. Conf Proc IEEE Eng Med Biol Soc 2009, 2332–2335 (2009).
16. Gopal, K. et al. Crystallographic protein model-building on the web. Bioinformatics 23, 375–377 (2007).
17. Romo, T. D., Sacchettini, J. C. & Ioerger, T. R. Improving amino-acid identification, fit and C αprediction using the Simplex method in automated model building. Acta Crystallogr D Biol Crystallogr 62, 1401–1406 (2006).
18. Gopal, K. et al. TEXTAL - Crystallographic protein model building using AI and pattern recognition. Ai Magazine 27, 15–24 (2006).
19. Gopal, K., Romo, T. D., Sacchettini, J. C. & Ioerger, T. R. Determining relevant features to recognize electron density patterns in x-ray protein crystallography. JOURNAL OF BIOINFORMATICS AND COMPUTATIONAL BIOLOGY 3, 645–676 (2005).
20. Gopal, K. et al. TEXTAL™: Automated Crystallographic Protein Structure Determination. 20, 1483 (2005).
21. Romo, T. D. et al. TEXTAL: AI-based structural determination for X-ray protein crystallography. IEEE INTELLIGENT SYSTEMS 20, 59–63 (2005).
22. Adams, P. D. et al. Recent developments in the PHENIX software for automated crystallographic structure determination. Journal of synchrotron radiation 11, 53–55 (2004).
23. Gopal, K., Romo, T. D., Sacchettini, J. C. & Ioerger, T. R. Efficient retrieval of electron density patterns for modeling proteins by X-ray crystallography. ICMLA (2004).
24. Gopal, K., Romo, T. D., Sacchettini, J. C. & Ioerger, T. R. Weighting features to recognize 3D patterns of electron density in X-ray protein crystallography. Proc IEEE Comput Syst Bioinform Conf 255–265 (2004).
25. Gopal, K., Pai, R., Ioerger, T. R., Romo, T. D. & Sacchettini, J. C. TEXTAL™: Artificial intelligence techniques for automated protein structure determination. 93–100 (2003).
26. Radding, W., Romo, T. D. & Phillips, G. N. Protein-assisted pericyclic reactions: An alternate hypothesis for the action of quantal receptors. Biophys J 77, 2920–2929 (1999).
27. Andrews, B. K., Romo, T. D., Clarage, J. B., Pettitt, B. M. & Phillips, G. N. Characterizing global substates of myoglobin. Structure 6, 587–594 (1998).
28. Romo, T. D., Clarage, J. B., Sorensen, D. C. & Phillips, G. N. Automatic identification of discrete substates in proteins: singular value decomposition analysis of time-averaged crystallographic refinements. Proteins 22, 311–321 (1995).
29. Clarage, J. B., Romo, T. D., Andrews, B. K., Pettitt, B. M. & Phillips, G. N. A sampling problem in molecular dynamics simulations of macromolecules. Proc Natl Acad Sci USA 92, 3288–3292 (1995).

CONFERENCE PUBLICATIONS

1. Gopal, K, Romo, TD, McKee, E, Childs, KC, Kanbi, L, Pai, R, Smith, J, Sacchettini, JC, Ioerger, TR. TEXTAL™: Automated crystallographic protein structure determination. IAAI-05 1483-1490 (2005).
2. Gopal, K, Romo, TD, Sacchettini, JC, Ioerger, TR. Efficient retrieval of electron density patterns for modeling proteins by X-ray crystallography. ICMLA-04 380-387 (2004).
3. Gopal, K, Romo, TD, Sacchettini, JC, Ioerger, TR. Weighting features to recognize 3D patterns of electron density in X-ray protein crystallography. IEEE CSB-04 255-265 (2004).
4. Gopal, K, Romo, TD, Sacchettini, JC, Ioerger, TR. Evaluation of geometric & probabilistic distance measures to retrieve electron density patterns for protein structure determination. ICAI-04 427-432 (2004).
5. Gopal, K, Pai, R, Ioerger, TR, Romo, TD, Sacchettini, JC. TEXTAL™: Artificial Intelligence Techniques for Automated Protein Structure Determination. IAAI-03 93-100 (2003)

TALKS & INVITED LECTURES

Spring, 2011 "NAMD on the BlueGene/Q" CIRC Workshop, Rochester, NY

Fall, 2010 "Multiscale Modeling of GPCRs" URMC Biochemistry Retreat, Rochester, NY

Spring, 2005 "The Simplex: Rigid-Body, Real-Space Refinement in LOOKUP." PHENIX International Meeting, Houston, TX.

Spring, 2004 "State of the Alignment". PHENIX International Meeting, Cambridge, UK

Fall, 2002 "Sequence Alignment in TEXTAL™." Third Tb Structural Genomics Consortium Retreat, Santa Fe, NM.

Fall, 2002 "Incorporating Sequence Alignment Methods into TEXTAL™." PHENIX International Meeting, College Station, TX.

Spring, 2002 "Aligning TEXTAL™." PHENIX International Meeting, Cambridge, UK.

Spring, 2002 "Crystallographic Refinement with TEXTAL™." Internet-2 Conference, IBT, Houston, TX

Fall, 2001 "Automating Refinement: The TEXTAL™ Perspective", IBT Seminar Series, Houston, TX.

Spring, 1998 "Identification and Modeling of Protein Conformational Substates." FSU Biological Sciences Departmental Talk, Tallahassee, FL.

Spring, 1996 "Protein Substate Modeling and Visualization Using the Singular Value Decomposition." NLM Trainees' Meeting, Bethesda, MD.

Spring, 1996 "Protein Substate Modeling and Identification Using the Singular Value Decomposition." Biophysical Society, Baltimore, MD.

Fall, 1995 "Protein Substate Modeling and Visualization in X-ray Crystallography." All-Texas Crystallography Conference, College Station, TX.

Fall, 1994 "The Singular Value Decomposition of Protein Conformations." World Congress on Computational Medicine and Public Health, Austin, TX.

OTHER PUBLICATIONS

Cover Art (2007) Handbook of Proteins, Structure, Function, and Methods, v2.

Romo, TD. (1997) *Hot Skill Sets (Essay)*. Special Issue on Bioinformatics - Science OnLine.

Conference Program & Visualization (1997) US/Japan Joint Seminar on Molecular Dynamics of Ligand Binding to Myoglobins and Related Heme Proteins.

Illustration (1997) Science News, v.150, p.212

Illustration (1997) Nature Biotechnology v.15, p.962

Cover (1996) 9th International Symposium on Bioluminescence and Chemiluminescence.

Cover of Computer Physics Communications (1995) v.91

Cover of Proteins (1995) v.22

SOFTWARE PACKAGES DEVELOPED

• LOOS	2008–2017	Lightweight Object Oriented Structure library (https://github.com/GrossfieldLab/loos)
• JTrak	2004-2006	An on-line database for tracking cloning pipeline progress and analysis of individual and aggregate performance data for the TBSGC (internal)
• iStitch	2002-2006	VR environment for detecting and correcting anomalous protein backbone chain connections modeled by CAPRA, part of the TEXTAL™ automated modeling system
• TAlign	2002-2006	Modified sequence alignment method for improving model-building results (part of TEXTAL™)
• TEXTAL	2001-2006	Core TEXTAL™ development, including software licensing system using public key cryptography; software distribution system; optimization for parallel IRIX

and PPC AltiVec; secondary structure prediction from structure; real-space refinement optimizations.

- iXrayView 1998-2001 Interactive VR simulation of an X-ray diffraction apparatus illustrating basic data-collection methods and the physics behind X-ray diffraction. Derived from XRayView, by George N. Phillips, Jr.
- iRibbons 1998-2003 VR interface added to Ribbons (derived from Ribbons by Mike Carson)
- PDBView 1998 Lightweight VR visualization and modeling system for crystallographic structures
- rTaenia 1998-1999 RenderMan-based system for creating animations visualizing the time-evolution of high-dimensional systems.
- XIsoserv 1996-1997 Adaptation of NCSA's IsoServ isosurface visualizer for use with X-ray crystallographic data, interfacing to both RenderMan and RMRibbons.
- RMRibbons 1995-1996 Pixar RenderMan support added to Ribbons (by Mike Carson) allowing high-quality rendering for print. Also included support for isosurface visualization, surface mapping of molecular properties, use of shaders to visualize additional properties, and support for display of vector fields.
- Taenia/Hydra 1994-1995 OpenGL software for visualizing time-evolution of high-dimensional systems & chaotic effects
- Sig/Sor 1992-1995 Parallel implementation of a Partial-SVD computation for very large matrices representing ensembles of protein conformations (built using ARPACK).

MAJOR PROGRAMMING LANGUAGES, PACKAGES, & LIBRARIES

C++/C	PERL	Python	Fortran
Swift/iOS	BASH	FORTH	Assembly
Matlab/Octave	Latex	Boost	NumPy
SWIG	Doxygen	Git/SVN	valgrind

HIGH PERFORMANCE COMPUTERS USED

SGI Power Challenge	TMC CM2a	Intel Delta	Intel Paragon
KSR-1	BlueGene/P	BlueGene/Q	