

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 α prediction 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 “NAMM on the BlueGene/Q” CIRC Workshop, Rochester, NY

Fall, 2010 “Multiscale Modeling of GPCRs” URM 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-I	BlueGene/P	BlueGene/Q	