

Reetal Pai

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Education:

Doctor of Philosophy in Computer Science, Jan 2002 – Present

Dissertation Topic: Structure to Function Relationship in Proteins: A Feature-Based Analysis
Texas A&M University, College Station, TX, USA (GPA: 3.8 / 4.0)

Master of Science in Computer Engineering, December 2001

Clemson University, Clemson, SC, USA
Thesis: “Automated Diagnosis of Retinal Images Using Evidential Reasoning” (GPA: 3.7 / 4.0)

Bachelor of Engineering in Electrical & Electronic Engineering, September 1998

University of Mysore, Mysore, India (GPA: 3.5 / 4.0)

Work Experience:

Research Assistant, Department of Biochemistry and Biophysics, Texas A&M University (May '07-Present)

- Developed computational biology tools for research related to *Mycobacterium tuberculosis* (Mtb)
- Worked with biochemists on developing strategies for inhibitor design using docking algorithms for various targets in Mtb
- Developed an interactive webtool that allows scientists in the TB community to experiment with various target selection criteria and explore ways to prioritize gene targets
- Configured and maintained scientific software packages
- Trained biochemists to use various computational data analysis software

Teaching Assistant, Department of Computer Science, Texas A&M University (Aug '06 – May '07)

- Aided in the development of assignments, exams and projects for an undergraduate introductory course in Artificial Intelligence

Summer Internship, Google Inc. (May '06 – Aug '06)

- Created a demo version of an attribute search tool for Google Base

Research Assistant, Department of Computer Science, Texas A&M University ('02 – May '06)

- Developed AI algorithms for TEXTAL and PHENIX crystallography packages
- Presented research at various regional, national and international conferences
- Aided in grant proposal preparation

Research Assistant, Department of Electrical & Computer Engg., Clemson University ('99 – '01)

- Developed AI algorithms for Structured Analysis of the Retina (STARE), a medical expert system
- Developed web-based tutorial for AI algorithms in STARE

Research Projects:

- **Dissertation Project**
 - Developing a feature-based analysis of the structure-function relationship in proteins
 - Developing an approach to deal with conformational flexibility present with large ligands
 - Developing various tools to analyse large amount of structural data available from the Protein Data Bank
 - Found conclusive evidence that the feature-based approach is a valid approach to the analysis of diverse active sites
- **Inhibitor design**
 - Worked with biochemists to explore possible inhibitors for various *M.tuberculosis* targets
 - Worked with DOCK6, OpenEye, CHARMM, Sybyl etc. to explore the various facets of protein-small molecule interaction
 - Developed a novel ranking function to reduce the number of false positives from large-scale virtual screens and increased recall by over 20% in test cases
- **Data mining software tool: Target Explorer**
 - Designed an interactive web site that allows the TB research community to experiment with different target selection criteria
 - Allows researchers to examine correlations between different sources of experimental data
 - Improves the turnabout time involved in analyzing different drug targets
 - Presently deployed on the TB website www.webtb.org
- **Automated Identification of Non-Crystallographic Symmetry**
 - Designed a brute-force algorithm that used local density calculations as a metric to identify NCS relationships
 - Improved time-performance of the brute-force algorithm significantly using a set of features based on electron density
 - Obtained operators with an accuracy comparable to and better than the operators obtained by existing methodologies
 - Developed a web-based interface for this algorithm
 - Python interface currently deployed in TEXTAL (an automated protein model building software) and PHENIX software packages
- **Automated Recognition of Co-Factor Binding Sites**
 - Designed a database containing examples of various co-factor binding sites ensuring diversity of example set
 - A feature-based approach to the identification and prediction of co-factor binding sites
 - Methodology had an accuracy of 85% when applied to four groups of co-factors
- **Stitch**
 - A fragment database approach to correcting chain breaks in the backbones built by TEXTAL
 - Stitch increased accuracy of the generated models on an average by 10-15%
 - Currently implemented as a part of TEXTAL and PHENIX software packages
- **Probabilistic approach to the prediction of side-chain identity**
 - Developed a multinomial approach to assessing side-chain identity based on the top 'k' matches obtained from a database search
 - Accuracy of methodology was equivalent to previous estimates based on local density correlations

- **STARE**
 - Designed and developed an automated diagnostic system using Bayesian reasoning to diagnose retinal images
 - Diagnostic system was able to differentiate between 13 diagnoses based on a probabilistic analysis with an accuracy of 75%

Publications:

- **Pai, R.**, Sacchettini, J.C. and Ioerger, T.R. Fragment-Based Analysis of Protein-Ligand Interactions Using Localized Stereochemical Features (Submitted to ISMB, Jan 2008).
- **Pai, R.**, Sacchettini, J.C. And Ioerger, T.R. Specificity Normalization for Identifying Selective Inhibitors in Virtual Screening (Submitted to BIOCOMP, Feb 2008)
- **Pai, R.**, Sacchettini, J.C. And Ioerger, T.R. Fragment-Based Analysis of Protein-Ligand Interactions Using Localized Stereochemical Features, (Accepted as a poster at RECOMB 2008)
- Gopal, K., McKee, E., Romo, T., **Pai, R.**, Smith, J., Sacchettini, J.C. and Ioerger, T.R. (2007). Crystallographic Protein Model-Building on the Web. *Bioinformatics*, 23:375-377.
- **Pai, R.**, Sacchettini, J.C. and Ioerger, T.R. (2006). Identifying Non-Crystallographic Symmetry in Macromolecular Electron Density Maps: A Feature-Based Approach. *Acta Cryst D*, Volume 62, Part 9, 1012-1021.
- Romo, T.D., Gopal, K., McKee, E., Kanbi, L., **Pai, R.**, Smith, J., Sacchettini, J.C., and Ioerger, T.R. (2005). TEXTAL: AI-based Structural Determination for X-ray Protein Crystallography. *IEEE Intelligent Systems*, 20(6): 59-63.
- Gopal, K., Romo, T., Mckee, E., Childs, K., **Pai, R.**, Smith, J., Sacchettini, J.C., Kanbi, L. and Ioerger, T.R. (2005) TEXTAL: Automated Crystallographic Protein Structure Determination. *IAAI*, 1483-1490.
- **Pai, R.**, Sacchettini, J. C. and Ioerger, T. R. Identifying Non-Crystallographic Symmetry: A Feature Based Approach. (2005) *XX Congress, International Union of Crystallography*
- Adams, P. D., Gopal, K., Grosse-Kunstleve, R. W., Hung, L. W., Ioerger, T. R., McCoy, A. J., Moriarty, N. W., **Pai, R.**, Read, R. J., Romo, T. D., Sacchettini, J. C., Sauter, N. K., Storoni, L. C., Terwilliger, T. C. (2004). Recent developments in the PHENIX software for automated crystallographic structure determination. *Journal of Synchrotron Radiation*, 11:53-55.
- Gopal, K., **Pai, R.**, Ioerger, T.R., Romo, T., and Sacchettini, J.C. (2003). TEXTAL: Artificial Intelligence Techniques for Automated Protein Structure Determination. *Proceedings of the Fifteenth Conference on Innovative Applications of Artificial Intelligence Conference (IAAI)*, 93-100
- **Pai, R.** Hoover, A. and Goldbaum, M. (2002) Automated Diagnosis of Retinal Images Using Evidential Reasoning, *15th International Conference on Systems Engineering, Las Vegas, NV*.
- **Pai, R.** (2001) Automated Diagnosis of Retinal Images Using Evidential Reasoning, M.S. Thesis, ECE Department, Clemson University.

Posters:

- **RECOMB, Singapore**, Fragment-Based Analysis of Protein-Ligand Interactions Using Localized Stereochemical Features, Mar 2008
- **Bioinformatics Workshop, Texas A&M University**, Fragment-Based Analysis of Protein-Ligand Interactions Using Localized Stereochemical Features, Feb 2008
- **Grace Hopper Conference, Orlando**, Feature-based Analysis of Protein Active Sites, Oct 2007
- **Grace Hopper Conference, San Diego**, Identifying Non Crystallographic Symmetry in Electron Density Maps: Artificial Intelligence Techniques in X-ray Crystallography, Oct 2006
- **International Union of Crystallography, Florence, Italy**, Identification of Non Crystallographic Symmetry, Aug 2005
- **Lost Pines, TX, Poster presentation**, The TEXTAL System: Artificial Intelligence Techniques for Automated Protein Model Building, Oct 2002

Presentations:

- **Grace Hopper Conference, San Diego**, Riding the Technology Wave: Computer Scientists Building a Better Tomorrow, *Panel Presentation*, Oct 2006
- **PHENIX, Houston, TX**, Identifying Non-Crystallographic Symmetry: A Feature Based Approach, Mar 2005
- **PHENIX, Texas A&M**, Stitch: A Bioinformatics Approach to joining CAPRA chains, Sep 2003
- **Texas A&M**, STARE: Automated Diagnosis of Retinal Images Using Evidential Reasoning, Jan 2002
- **Journal Club, Texas A&M**
 - i. Seminar Presentation on the Structure-Function Relationship in Human Tissue Plasminogen Activator (Therapy for Heart Attacks and Strokes), Oct 2007
 - ii. Seminar Presentation on “Structural Similarity Enhances Interaction Propensity of Proteins”, Feb 2007
 - iii. Seminar Presentation on “From protein structure to biochemical function?”, Oct 2006
 - iv. Seminar Presentation on “Novel Statistical-Thermodynamic Methods to Predict Protein-Ligand Binding Positions Using Probability Distribution Functions”, Feb 2006
 - v. Seminar Presentation on “Protein Function Prediction Using Local 3D Templates”, Aug 2005
 - vi. Seminar Presentation on “Anatomy of protein pockets and Cavities: Measurement of Binding Site Geometry and Implications to Ligand Design”, Feb 2005

Software Development:

- Participated in the design and implementation of TEXTAL, a commercially available automated protein model building software
- Implemented TEXTAL tasks for PHENIX, an automated X-ray crystal structure determination software

- Created a web-based algorithm, PRANCS, to identify NCS relationships in electron density maps using a pattern recognition approach
- Developing a web based report system for Brazos County Rape Crisis Center
- Developed an interactive web based tool (Target Explorer) presently used by scientists in the Tuberculosis community (www.webtb.org)
- Program development in C and Python

Activities and Leadership Roles:

- Participant, Grace Hopper Conference, Oct 2007 (Volunteer, Registration Grant received)
- Google Ambassador Aug 2006 – Present
- AWICS Mentoring Officer Aug 2006 – Present, Distinguished Lecture Officer 2004 – 2006
- Participant, Grace Hopper Conference, Oct 2006 (All expenses scholarship received)
- Reviewer, *Frontiers in Education* 2006
- Participant, Google Workshop for Women Engineers, Jan 2006
- Volunteered at ISMB Conference, Detroit, Michigan July 2005 (Registration grant received)
- Participant, IUCR Conference, Florence, Italy Aug 2005 (Registration and accommodation grant received)
- Department of Computer Science Mentor 2005 – Present
- Participant, Graduate Teaching Academy 2005 – Present
- Computer Science Graduate Student Association (CSGSA) President 2005 – 2006 (Awarded the Graduate Leadership Award)
- Volunteer, Brazos County Rape Crisis Center 2004 – Present (Awarded the Volunteer of the Year for 2005, 2006)
- Computer Science Departmental Scholarship 2004
- Participant, 3 Workshops held as a part of the Gender Equity Project 2003 – 2004

References:

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