

# SABAREESH SUBRAMANIAM

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## Areas of Interest

Computational protein modeling, structural bioinformatics, object-oriented design, algorithms, machine learning, computer architecture, operating systems and multicore programming.

## Education

### **University of Wisconsin-Madison, USA**

PhD in Computational Biology, expected December 2013

Advisor: Alessandro Senes

Thesis: *Methods for 3D structure prediction of trans-membrane proteins(tentative).*

### **University of Wisconsin-Madison, USA**

GPA: 3.73/4.0

M.S. in Computer Sciences, May 2010

Courses: *Artificial Intelligence, Computer Architecture, Operating Systems, Algorithms.*

### **PSG College of Technology, Anna University, India**

GPA: 9.51/10.0

B.E Electronics and Communication Engineering, July 2006

## Positions

2008-current	Research Assistant, Biochemistry, University of Wisconsin-Madison, USA.
2009	Software Engineering Intern, Qualcomm Inc., San Diego, USA.
2006-08	Software Engineer, Cisco Systems Inc., Bangalore, India.
2006	Project Intern, Cisco Systems Inc., Bangalore, India.

## Skills

- Seven years of **C/C++** programming experience in a Linux environment.
- **Open-source** developer - [MSL](#)
- Currently administer the senes lab computational cluster.
- Fluent Perl programmer.
- Applied machine learning.
- Significant experience with core Java, Python, Tcl and MATLAB.
- Course work in multicore programming.

## Courses at University of Wisconsin-Madison

Introduction to Computer Architecture (CS/ECE 552)  
Introduction to Operating Systems (CS 537)

Introduction to Computer Networks (CS 640)  
Advanced Computer Architecture (CS/ECE 752)  
Multicore Programming (CS 758)  
Advanced Operating Systems (CS 736)  
Machine Learning (CS 760)  
Advanced Methods in Artificial Intelligence (CS 731)  
Advanced Natural Language Processing (CS 769)  
Introduction to Bioinformatics (CS 576)  
Introduction to Algorithms (CS 577)  
Protein and Enzyme Structure and Function (BIOCHEM 601)  
Introduction to Statistical Inference (STAT 610)

## **Publications**

- **Subramaniam S** and Senes A "[An Energy-Based conformer library for side chain optimization: improved prediction and adjustable sampling](#)", Proteins 2012
- Kulp DW, **Subramaniam S**, Donald JE, Hannigan BT, Mueller BK, Grigoryan G and Senes A "[Structural informatics, modeling and design with an open-source Molecular Software Library \(MSL\)](#)", J Comput. Chem. 2012
- **Subramaniam S**, Natarajan S, and Senes A "A Machine Learning based Approach to improve Protein Sidechain Optimization", ACM Conference on Bioinformatics, Computational Biology and Biomedicine (ACM BCB) 2011, p478-480
- LaPointe L, Taylor K, **Subramaniam S**; Khadria A, Rayment I, Senes A "[Structural organization of FtsB, a transmembrane protein of the bacterial divisome](#)", Biochemistry 2013
- **Subramaniam S** and Senes A "A backbone-dependant energy-based conformer library improves sidechain optimization", *in preparation*.
- **Subramaniam S\***, Mueller BK\*, Senes A "[CATM: High resolution structure prediction of trans-membrane helical dimers](#)" *in preparation*.

## **Talks**

- CIBM Seminar (BMI 915) September 20, 2011. "[Efficient Conformer Libraries to improve sidechain optimization.](#)"
- IPIB Seminar March 30, 2012. "[Predicting Protein Sidechain Conformations - A New Strategy.](#)"
- From Computational Biophysics to Systems Biology May 19, 2013. "[Structure Prediction of Transmembrane Helix Association](#)".

## **Research Experience**

**University of Wisconsin-Madison**, Department of Biochemistry  
**Research Assistant**, September 2008-present

Developing computational methods for protein modeling and structural analysis with emphasis on improving **sidechain optimization** and **structure prediction of trans-membrane proteins**.

Developing a C++ library called MSL for modeling protein molecules, available online at <http://www.msl-libraries.org>.

## **Professional Experience**

**Qualcomm Inc.**, San Diego, CA  
**Interim Engineering Intern**, LTE - L1 Modem SW group May 2009 - Aug 2009

Developed a framework using **C++/XML** data binding to test connected mode measurement reporting on LTE systems.

Profiled the Inter Processor Message transfer mechanism (part of the firmware driver) on the LTE systems.

**Cisco Systems Inc.**, Bangalore, India  
**Project Intern**, November 2005 - May 2006  
**Software Engineer**, July 2006 - July 2008

Developed **C/C++** software for Cisco ONS15xxx range of optical switching devices.  
Developed a **TCL/Expect** based test automation suite.

## **Open source Project**

### **Molecular Simulation Library (MSL)**

MSL is an open-source **C++** library for molecular modeling, analysis and design developed by a small group of collaborators. The core objects in MSL are about 100,000 lines of C++ code with about 160 classes. These classes provide functionality of varying complexity; ranging from simple functions like measuring distances and angles between atoms, to geometric transformations of molecules; complex sidechain optimization algorithms and energy minimization routines. Open source libraries such as the [GNU Linear Programming Kit \(GLPK\)](#) and [GNU Scientific Library](#) have been leveraged to implement sidechain optimization and energy minimization respectively.

Most of my time is spent either enhancing MSL or writing protein modeling applications using MSL. It is free for download at [sourceforge](#). You can find more details [here](#).

## Research Projects

### Transmembrane dimers with C $\alpha$ -mediated hydrogen bonding (CATM)

CATM is an MSL program that predicts how two helical protein segments would associate to form a symmetric homodimer in a membrane environment. It is fundamentally, a search over the space (3 rotational and one translational degrees of freedom) of dimer geometries for structures with favorable energy scores. The search is made tractable by imposing geometric constraints derived from biochemical principles and other sequence-specific analysis.

We have achieved enough efficiency to be able to scan entire genomes on our 128-node computational cluster. Infact, we have applied CATM to all predicted [transmembrane proteins](#) in the human genome and the results are available [here](#). The entire run, scanning about 2300 proteins takes about 2-3 days.

### Energy-based protein sidechain conformation libraries (EBL and BEBL)

[Sidechain optimization](#) is an important component of any protein design or structure prediction method. Each position on the given protein backbone is allowed a set of discrete representative geometries or conformations called a conformer or rotamer library. The individual positions are allowed to assume conformations independent of other positions and this combinatorial space is searched for the configuration (one conformation per position) with the lowest energy. The search is performed via popular algorithms (***greedy trials, dead end elimination, monte carlo simulated annealing, linear programming, self-consistent mean field***) implemented in MSL.

The conformer library is typically created using some kind of geometric clustering, however, we have created an energy-based method based on importance sampling, to compile more efficient conformation libraries. This library, called the [EBL](#) outperforms all popular sidechain libraries in terms of efficiency(speed) as well as accuracy of prediction. We have created both backbone-dependent as well as backbone-independent libraries and use them extensively in all our protein modeling applications.

## Test Scores

**GRE 2006 - 1500/1600**

**TOEFL 2007 – 112/120**

## **REFERENCES**

Available on request.