

## CURRICULUM VITAE

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### **Education:**

B.Sc. University of Pune, April, 1984  
M.Sc. University of Pune, April, 1986  
Ph.D. University of Pune, Department of Chemistry, Nov, 1993

### **Programming Skills:**

Languages: FORTRAN, Awk, Perl, C++  
Operating Systems: MS-DOS, Windows, Unix, Linux  
PLATFORMS: HP9050, PARAM (64-node parallel machine), Iris, Indigo, RISC 6000, DEC-10000, SP2, SGI-O2, OSCAR (84-node SGI Cray Origin 2000 parallel machine with R10000 processors, BIOWULF(AMD XP/Athlon Cluster)

### **Scientific Software Used:**

Ab Initio: Micromol, Gaussian96,,Gamess  
Molecular Dynamics: CharmM, Gromacs, NAMD  
Molecular Graphics: Quanta, Insight-II, Rasmol, Molscript, Raster-3D, Povray,  
Sequence Alignments: BLAST, FASTA, ClustalW  
Structure Prediction : Memsat, PHDhtm, DAS, TMAP, TMPRED,  
Homology Modeling : Modeller4, Look  
Coarse grained Modeling: GNM, ANM

### **Software Development:**

Was a Team member from the University of Pune, India (headed by Prof. S.R. Gadre), which developed the program INDMOL, a package to generate ab initio molecular wave functions, which is being marketed by Center of Development of Advanced Computing, (C-DAC), India.

### **Brief Chronology of Employment:**

1987 - 1989 - Junior Research fellow, University of Pune, India.  
1989 - 1992 - Senior Research fellow, University of Pune, India.  
1992 - 1994 - Research Associate, C-DAC, Pune, India.

- 1994 - 1996 - Indian Institute of Science, Bangalore, India.
- 1996 - 1998 - Alexander Humboldt Fellow, EMBL, Germany.
- 1998 - 2001 - Post-Doctoral Fellow, University of Oxford, Laboratory of Molecular Biophysics, Oxford, UK
- 2001 - 2004 - Fogarty Visiting Fellow, LECB, NIH, USA.
- 2004 - present - Research Associate at Department of Computational Biology, Pittsburgh, PA.

**Society membership:**

- Biophysical Society, 1998 – Present
- Federation of American Societies for Experimental Biology (FASEB) 2002 – Present

**Honors & Other Special Scientific Recognition:**

- The National Open Merit Scholarship for Graduate and post-graduate studies in India, 1979-1986.
- University Grants Commission (UGC) Research Fellowship by the Government of India, 1988-1992.
- Post-Doctoral Fellowship, Center for Development of Advanced Computing, India, 1992-1994. The PARAM Awards, Center for Development of Advanced Computing, India, 1993.
- Post-Doctoral Fellowship, Department of Biotechnology, India, 1994-1996.
- Alexander van Humboldt Post-Doctoral Fellowship, 1996-1998.

**Research Experience:**

**2004 to Present:**

Research associate at the Department of Computational Biology, in Pittsburgh with Prof Iveta Bahar. Here I am applying Gaussian Network Models to predict the conformational changes associated with functional transitions in membrane proteins.

**2001 to 2004:**

Research associate at the National Institute of Health, Maryland, in the Laboratory of Experimental and Computational Biology, with Dr H Robert Guy. Application of molecular modeling and molecular dynamics simulations to validate and refine homology and structural models of membrane proteins.

**1998 to 2001:**

Post-Doctoral Fellow at Laboratory of Molecular Biophysics, Oxford, UK with Professor MSP Sansom. Learned and applied molecular dynamics simulations to investigate the gating mechanism of the first potassium channel to be crystallized, KcsA.

**1996 to 1998:**

I worked at EMBL in Rebecca Wade's group, as an Alexander von Humboldt post-doctoral fellow. Studied role of salt-bridges in stabilizing thermophilic and mesophilic proteins.

**1994 to 1996:**

Post-doctoral fellow at Indian Institute of Science, with Prof Saraswati Vishweshwara. I developed a FORTRAN code to carry out Monte Carlo simulations on a cubic lattice, in order to study the energy landscape of folding of homopolymer.

**1986 to 1994:**

Department of Chemistry, University of Pune, with Prof SR Gadre. My doctoral thesis work was on the Quantum and Computational Chemistry, I developed and optimized a FORTRAN code for the computation of molecular electrostatic potential from ab initio wave functions.

**Symposium/Seminars Presentations:**

Flexibility in Biomolecules, Arizona, 2005.  
Biophysical Society, Baltimore, Maryland, 2004  
Biophysical Society, San Antonio, Texas, 2003.  
Biophysical Society. San Francisco, California, 2002.  
Structural Genomic Meeting. Cambridge, MA., 2000.  
European Biophysical Meeting. Munich, FRG., 2000.  
Structure, Dynamics and Perturbations of Membranes Symposium. Chester, UK, 2000.  
18<sup>th</sup> International meeting of the Molecular Graphics & Modeling Society. York, UK., 2000.  
Meeting of the Physiological Society, University of Newcastle-upon-Tyne, UK, 1999.  
XIII<sup>th</sup> International Biophysics Congress. New Delhi, India, 1999.  
XIII<sup>th</sup> International Biophysics Congress on Membranes. Hyderabad, India 1999.  
Biophysical Society, Baltimore, MD., 1999.  
Faraday Discussion No. 111, Molecular Interactions of Biomembranes, Bristol, UK, 1998.  
Novartis Foundation meeting for Gramicidin and Related ion Channel forming peptides. London, UK., 1998.

**Invited Talks:**

The 3rd Annual Biological Language Conference, Pittsburgh, November 2005.  
Center for Computational Biology and Biophysics, Pittsburgh, September 2004  
University of Oxford, UK, October, 2001  
Centre for Cellular and Molecular Biology, Hyderabad, India, June, 2001  
Molecular Biophysics Unit, Indian Institute of Science, Bangalore, India, June, 2001  
Institute of Microbial Technology, Chandigarh, India, June, 2001  
University of Birmingham, UK, August, 2000.