Summary Curriculum Vitae of

Sagar A. Pandit

Summary:

Publications:

Total publications	43
Number of invited reviews	2
Number of book chapters	5
Number of peer reviewed papers	35
Number of citations	~1700
H-index	21

Funding:

Total external funding: $476,304 (My Share)

1. NIH Grant 1R01GM086707–01A1, Co-PI, My Share: $397,072
2. DOE Grant, DE-FC52-08NA28617. , Co-PI, My Share: $79,232

Total internal funding: $5000

Teaching: Total first time courses taught: 8

Service: Departmental colloquium chair, Served on departmental search committee. CAS computational committee, CAS faculty development committee. Other professional services.

Basic Information

Name: Sagar Avinash Pandit
Address:
Department of Physics,
University of South Florida,
4202 E Fowler Ave, PHY 114,
Tampa, FL 33620
Phone: (813) 974 2781 (Office), (765) 337 3399 (Cell)
E-mail: pandit@usf.edu
Home page: https://csmlabfs1.cas.usf.edu/Sites
Basic areas of interest:
Computational Biophysics, Complex Systems, Dynamical systems, Computer Science.

Academic Qualification

Ph.D.:
Ph. D. (Physics), 1999 from
Department of Physics, University of Pune, Pune, India.
Thesis title:
Geometric formulation of Generalized Nambu systems and its applications.
M. Sc.:
M. Sc. (Physics), 1991 from
Department of Physics, University of Pune, Pune, India. I Class with distinction
B. Sc.:
B. Sc. (Physics), 1989 from
Parle College, University of Bombay, Mumbai, India. I Class

Awards

★ Post Doctoral Fellowship at the Physical Research Laboratory, Ahmedabad, India for the period Oct. 1998 to Sept 2000.
★ Council for Scientific and Industrial Research (CSIR) fellowship for the period Sept. 1992 to Oct. 1997 during Ph.D. and qualified the National Eligibility Test (NET), India.
★ Qualified Graduate Aptitude Test in Engineering (GATE) (Physics), India in 1991 with percentile score 96.83.
★ University Grant Commission (UGC) fellowship for the period 1989-1991 for M. Sc. at the Department of Physics, University of Pune, Pune, India.
★ A gold medal in National Graduate Physics Examination in 1989 conducted by Indian Association of Physics Teachers (IAPT) at the national level.

Professional Experience

★ **Aug. 2013 – :** Associate Professor, Department of Physics, University of South Florida, FL.
★ **Aug. 2007 – Aug. 2013:** Assistant Professor, Department of Physics, University of South Florida, FL.
★ **Oct. 2005 – Jul. 2007 :** Research Associate, Department of Computer Science, Purdue University, IN
★ **July 2003 - Oct. 2005 :** Senior Research Associate, Illinois Institute of Technology, IL
★ **Oct. 2000 - June 2003 :** Research Associate, Department of Chemistry, University of North Carolina, NC
★ **Oct. 1998 - Oct. 2000 :** Post Doctoral Fellow, Physical Research Laboratory, Ahmedabad, India.
★ **Oct. 1997 - Sept. 1998 :** Systems and network administrator at the Center for Network Computing, University of Pune, Pune, India.
★ **Sept. 1992 - Sept 1999 :** Ph. D. studies, thesis title Geometric formulation of Generalized Nambu systems and its applications , at the Department of Physics, University of Pune, Pune, India.
★ **August 1991 - Sept. 1992 :** Attended graduate courses in Astrophysics at Inter University Center for Astronomy and Astrophysics (IUCAA), Pune, India.

Meetings, Schools, Workshops, and Conferences

★ The Annual Biophysical Society Meeting at the Baltimore convention center, Baltimore, USA in Mar 2011.
★ The Annual Biophysical Society Meeting at the Boston convention center, Boston, USA in Feb 2009.
★ The Annual Biophysical Society Meeting at the Long beach convention center, Long beach, USA in Feb 2008.
★ “Biological Membranes and Membrane Proteins: Challenges for Theory and Experiment” at the Park City, Utah, June 10-14, 2007.
★ The Annual Biophysical Society Meeting at the Baltimore convention center, Baltimore, USA in Mar 2007.
★ The Annual Biophysical Society Meeting at the Salt Lake city convention center, Salt Lake city, USA in Feb 2006.
★ The Annual Biophysical Society Meeting at the Long Beach convention center, Long Beach, USA in Feb 2005.
★ The Annual Biophysical Society Meeting at the Baltimore convention center, Baltimore, USA in Feb 2004.
★ The Annual Biophysical Society Meeting at the Gonzales convention center, San Antonio, USA in Feb 2003.
★ The Annual Biophysical Society Meeting at the Mascone convention center, San Francisco, USA in Feb 2002.

★ The “International summer school on Statistical Physics and Probabilistic Methods in Computer Science” at The International Center for Theoretical Physics, Trieste, Italy held in August 1999.
★ The “International conference on Dynamical Systems” at the Indian Institute of Sciences (IISC), Bangalore, India held in Jan, 1997 organized by Department of Mathematics, IISC.
★ “Frontier Lectures in Condensed matter Sciences” at the Department of Physics, University of Pune, Pune, India, held in 1997 organized by Jawaharlal Nehru Center (JNC) Bangalore, India.
★ A workshop-cum-tutorial “Parallel computing in Science and Engineering” at Center for Development of Advance Computers (C-DAC), Pune, India, held in June, 1996 organized by C-DAC.
★ A workshop on “Computer Networks” at Inter University Center for Astronomy and Astrophysics (IU- CAA), Pune, India, held in 1994 organized by IUCAA and National Center for Software Technology (NCST), Mumbai, India. Conducted lab tutorials in this workshop
★ A school on “Manifolds and Physics” at Thiruchirapalli in 1993 organized by Bharathidasan university and National Board of Higher Mathematics (NBHM),India.

Teaching Experience

★ **PHY-6536:** *Statistical Physics* for the Physics graduate students at the University of South Florida.
★ **PHZ-5156C:** *Computational Physics* for the Physics graduate students at the University of South Florida.
★ **PHY-5937:** *Introduction to Computational Physics* for Physics graduate students at the University of South Florida.
★ **PHY-4523:** *Statistical Mechanics* for Physic undergraduate students at the University of South Florida.
★ **PHY–4604:** *Introduction to Quantum Mechanics* for the Physics under–graduate students at the University of South Florida
★ **PHY–2048:** *General Physics I* for the freshman at the University of South Florida.
★ **PHY–2102:** *General Physics Problems* for the freshman at the University of South Florida.
★ **PHY–4702:** *Applications of Physics to Biology and Medicine I* for pre–medical freshman at the University of South Florida.
★ **PHY–4703:** *Applications of Physics to Biology and Medicine II* for pre–medical freshman at the University of South Florida.
★ **PHY–4151C:** *Computational Physics* for the Physics under–graduate students at the University of South Florida
★ **PHYS–304:** *Kinetic Theory & Thermodynamics* for the Physics undergraduate students at the Illinois Institute of Technology, Chicago, IL (Spring 2005). The course is based on books i) Equilibrium thermodynamics by C. J. Adkins, ii) Thermodynamics, Kinetic Theory, and Statistical Thermody- namics by F. W. Sears, G. L. Salinger.

★ **PHYS–508:** *Analytical dynamics* for the Physics graduate students at the Illinois Institute of Technology, Chicago, IL (Fall 2004). The course is based on books i) Classical Dynamics: A contemporary approach, by J. V. Jose´ , E. J. Saletan, ii) Introduction to mechanics and symmetry, by J. E. Marsden, T. S. Ratiu, and iii) Classical mechanics, by H. Goldstein.
★ A course titled Numerical methods in classical mechanics for the college teachers under the College Teacher's Training Program at the Physical Research Laboratory, Ahmedabad, India (August 2000) . The course was centered around the various numerical methods to solve initial value problems.
★ A course titled *Radiosity* for graduate (M.C.A.(VI semester)/M.Sc.(IV semester)) students at the Department of Computer Science, University of Pune, Pune, India (Semester IV of Indian academic year 1997-98) . The course was centered around global illumination models, emphasizing the Radiosity method.
★ A course on C++ at the Center for Network Computing, University of Pune, Pune, entitled *Object based programming in C++: A paradigm perspective* (1997). Various programming paradigms were discussed in this course.

Computational Skills

Scientific Computing

★ On going development of automatic force field optimization tool FFOpt.
Language: C
★ On going development of molecular dynamics package with reactive force fields.
Language: C
★ On going development of Semigrand Gibbs Ensemble Monte Carlo simulation code and an interface for this code to the GROMACS system.
Language: C
★ Experience in molecular mechanical modeling with the existing software packages such as Gaussian (for QM/MM modeling), GROMACS (MD and energy minimization), AMBER, APBS (Poisson–Boltzmann solver).
★ Modifications to the open source software GROMACS to improve performance of Particle Mesh Ewald sum (PME) calculations. (2004 – 2005)
★ Developed a set of tools to modify and analyze the topologies of complex molecules. This toolbox also includes tools for analysis of molecular dynamic trajectories. Some of the recent algorithms are implemented (developed during Nov 2000 – present).
Language: C++
★ Monte Carlo simulations of the model systems describing bio-membrane : Developed and im- plemented Monte Carlo simulations for the system of disks of various shapes interacting via given potential. The results of such simulations are compared with experimental results for real liposome membranes (developed in 1997).
Language: C++
See (http://xxx.lanl.gov/abs/cond-mat/0002148, http://xxx.lanl.gov/abs/physics/9903012)
★ Graph Tools : Implemented various algorithms for graphs. e.g. : Least path, Characteristic length of a graph calculation of clique and other statistical properties like average in degree, out degree etc (developed during 1998 – 1999).

Language: C++
See (http://xxx.lanl.gov/abs/chao-dyn/9901017, http://xxx.lanl.gov/abs/cond-mat/0004163)
★ Diagonalisation of large matrices (Sparse) : Implemented Householder algorithm for diagonli- sation of large sparse matrices. The sparse matrix can be represented in either Row index form or Column index form (developed for the Quantum chaos group at the Physical Research Laboratory in 1998).
Language: C.

Systems Administration

Installation and Systems/network administration of WAN at the University of Pune, India. Experience of various dialects of UNIX. (e.g. Linux, Solaris, IRIX, HPUX, AIX, MacOS X etc.) and TCP/IP based wide area network (Campus wide optic fiber) (1997–1998).
Administration and installation of 10 nodes linux cluster at the laboratory of Prof. H. L. Scott, Illinois Institute of Technology, Chicago (from 2003).

Publications and Preprints

Total citation index: **~1700** H-index: **21**
Google scholar profile: http://scholar.google.com/citations?user=o-FxB9wAAAAJ&hl=en

Book chapters and reviews:

1. ***N–body computational methods,***
   Joseph C Fogarty, Hasan Metin Aktulga, Sagar A Pandit, and Ananth Y Grama
   Springer's Encyclopedia of Parallel Computing, 2011
2. ***Multiscale simulations of heterogeneous model membranes,***
   Sagar A. Pandit, and H. L. Scott
   Biochimica et Biophysica Acta 1788, 136–148, 2009
3. ***Atomistic and Mean Field Simulations of Lateral Organization in Membranes***
   Sagar A. Pandit, See-wing Chiu, Eric Jakobsson and H. Larry Scott
   Chapter 10 of Current Topics in Membranes, Volume 60, edited by Scott Feller, 2008
4. ***Simulations and Models of Lipid Bilayers***
   Sagar A. Pandit, and H. L. Scott
   Chapter 2 of Soft Matter – vol. 4, eds. Gerhard Gompper and Michael Schick, 2008.
5. ***Atomistic and coarse-grained computer simulations of raft-like lipid mixtures,***
   Sagar A. Pandit, and H. L. Scott
   Chapter 19 of Methods in Molecular Biology, vol 398: Lipid Rafts, ed. Tom McIntosh, 2008.
6. ***Aqueous Solutions next to Phospholipid Membrane Surfaces: Insights from Simulations,***
   Max L. Berkowitz, David L. Bostick and Sagar A. Pandit
   Chemical Reviews, 106, 1527–1539, 2006.
7. ***Towards a general model for male–male coalitions in primate groups,***
   Carel P. van Schaik, Sagar A. Pandit, Erin Vogel,
   Chapter in Cooperation in primates, ed. P. M. Kappeler, Carel P. van Schaik, Springer Verlag, Berlin, 2005.

Peer Reviewed articles:

8. **Why do chimpanzee males attack the females of neighboring groups?**
   G. R. Pradhan, Sagar A. Pandit, Carel van Schaik
   (In communication with the American Journal of Physical Anthropology)
9. **DCMS: A System for Molecular Simulation Database Management**
   Anand Kumar, Vladimir Grupcev, Meryem Berrada, Yi-Cheng Tu, Sagar Pandit, Xingquan Zhu, Joseph Fogarty, Yuni Xia
   (Accepted for the International Coneference on Statistical and Scientific data management)
10. **Automated Optimization of Water-Water Interaction Parameters for a Coarse-Grained Model**
    JC Fogarty, SW Chiu, P Kirby, E Jakobsson, Sagar A Pandit
    J. Phys. Chem. B, 118 (6), pp 1603–1611, 2014.

11. **Approximate algorithms for computing spatial distance histograms with accuracy guarantees**
V Grupcev, Y Yuan, YC Tu, J Huang, S Chen, Sagar A Pandit, M Weng
Knowledge and Data Engineering, IEEE Transactions on 25 (9), 1982-1996, 2013.
12. ***A lattice model of cross-linked polymeric materials: the role of randomness***
C. Brad Bennett, James Kruczek, D. A. Rabson, W. Garrett Matthews, Sagar A. Pandit
Journal of Physics: Condensed Matter 25 (28), 285101, 2013.
13. ***Compression in Molecular Simulation Datasets***
Anand Kumar , Xingquan Zhu , Yi-Cheng Tu , Sagar Pandit
Accepted for publication in International Journal of Advancements in Computing Technology, 2012.
14. ***On Fast Algorithms for Computing Spatial Distance Histograms***
Vladimir Grupcev, Yongke Yuan, Yi-Cheng Tu, Jin Huang, Shaoping Chen, Sagar A Pandit, and Michael Weng
Accepted for publication in Transactions on Knowledge and Data Engineering, 2012.
15. ***Mixing Properties of Sphingomyelin Ceramide Bilayers: A Simulation Study***
Rainer Metcalf, and Sagar A Pandit
J. Phys. Chem B, 116, 4500-4509, 2012
16. ***Reactive Molecular Dynamics: Numerical Methods and Algorithmic Techniques***
Hasan Metin Aktulga, Sagar A. Pandit, Adri C. T. van Duin, and Ananth Y Grama
SIAM J. Sci. Comput. Vol. 34, No. 1, pp. C1–C23, 2012.
17. ***Parallel reactive molecular dynamics: Numerical methods and algorithmic techniques***
Hasan Metin Aktulga, Joseph C. Fogarty, Sagar A Pandit, and Ananth Y Grama
Parallel Computing 38, 245–259, 2012.
18. ***Self-consistent mean-field model for palmitoyloleoylphosphatidylcholine–palmitoyl-sphingomyelin–cholesterol lipid bilayers***
Paul W Tumaneng, Sagar A Pandit, Guijun Zhao, and H. L. Scott
Phys Rev E **83**, 031925, 2011
19. ***Mating strategies in primates: A game theoretical approach to infanticide***
James E Lyon, Sagar A Pandit, Carel P. van Schaik, and Gauri R. Pradhan
Journal of Theoretical Biology 274, 103–108, 2011
20. ***A reactive molecular dynamics simulation of the silica-water interface***
Joseph C. Fogarty, Hasan Metin Aktulga, Adri van Duin, Ananth Grama, and Sagar A. Pandit
J. Chem. Phys.,132, 174704, 2010
21. ***Lateral Organization of Complex Lipid Mixtures from Multi-scale Modeling,***
Paul W. Tumaneng, Sagar A. Pandit, Guijun Zhao, and H.L. Scott
J. Chem. Phys., 132, 065104, 2010
22. ***An improved united atom force field for simulation of mixed lipid bilayers,***
See-Wing Chiu, Sagar A. Pandit, H. L. Scott, and Eric Jakobsson
J. Phys. Chem. B 113 (9), 2748–2763, 2009
23. ***Computing Spatial Distance Histograms Efficiently in Scientific Databases,***
Yi-cheng Tu, Shaoping Chen, and Sagar A. Pandit

Proceedings of the 25th IEEE Intl Conference on Data Engineering (ICDE), DOI 10.1109/ICDE.2009.30, 2009

24. ***Cholesterol Packing around Lipids with Saturated and Unsaturated Chains: A Simulation Study,***
Sagar A. Pandit, See-Wing Chiu, Eric Jakobsson, Ananth Grama, and H. L. Scott
Langmuir 24, 6858–6865 2008
25. ***Cholesterol surrogates: a comparison of cholesterol and 16:0 ceramide in POPC bilayers,***
Sagar A. Pandit, See–Wing Chiu, Eric Jakobsson, Ananth Grama, and H. L. Scott
Biophys. J., 92, 920–927, 2007
26. ***Lateral Organization in lipid-cholesterol mixed bilayers,***
Sagar A. Pandit, George A. Khelashvili, Eric Jakobsson, Ananth Grama, and H. L. Scott
Biophys. J., 92 (2), 440–447 2007.
27. ***Molecular Dynamics Simulations of Reactive Systems,***
Sagar A. Pandit, Metin Aktulga, and Ananth Y. Grama
Appears in mini symposium on the Parallel Matrix Algorithms and Applications, 2006.
28. ***Molecular Dynamics Simulation of a Ceramide Bilayer***
Sagar A. Pandit, H. Larry Scott
J. Chem. Phys, 124, 014708, 2006.
29. ***Self-Consistent mean field model based on Molecular Dynamics: Application to Lipid-Cholesterol Bilayers,***
George A. Khelashvili, Sagar A. Pandit, H. L. Scott,
J Chem Phys, 123, 034910, 2005.
(ALSO APPEARS IN THE AMERICAN PHYSICAL SOCIETY VIRTUAL JOURNAL OF BIOLOGICAL PHYSICS RE- SEARCH 10(3), (2005))
30. ***Simulation of the early stages of the nano–domain formation in Mixed bilayers of Sphingomyelin, Cholesterol and Dioleylposphatidylcholine,***
Sagar A. Pandit, Eric Jakobsson, H. L. Scott,
Biophys J, 87(5), 3312–3322, 2004.
31. ***Sphingomylin–Cholesterol domains in phospholipid membranes: Atomistic simulation,***
Sagar A. Pandit, S. Vasudevan, S. W. Chiu, R. J. Mashl, Eric Jakobsson, H. L. Scott
Biophys J, 87(2), 1092-1100 2004.
32. ***A model for within–group coalitionary aggression among males***
Carel P. van Schaik, Sagar A. Pandit, Erin Vogel
Behavioural Ecology and Sociobiology 57, 101–109, 2004.
33. ***Complexation of Phosphatidylcholine Lipids with Cholesterol,***
Sagar A. Pandit, David Bostick, Max L. Berkowitz,
Biophys J, 86(3), 1345–1356 2004.
34. ***Mixed Bilayer Containing Dipalmitoylphosphatidylcholine and Dipalmitoylphosphatidylserine: Lipid Complexation, Ion Binding, and Electrostatics***
Sagar A. Pandit, David Bostick, Max L. Berkowitz
Biophys J, 85(5), 3120–3131, 2003.

35. ***A model for leveling coalitions among primate males: Toward a theory of egalitarianism***
Sagar A. Pandit, Carel P. van Schaik
Behavioural Ecology and Sociobiology 55, 161–168, 2003.

36. ***An Algorithm to Describe Rugged Molecular Interfacial Surfaces and its Application to a Study of Water at the Lipid Bilayer Interface***
Sagar A. Pandit, David Bostick, Max L. Berkowitz,
J Chem Phys, 119(4), 2199–2205, 2003.
(ALSO APPEARS IN THE AMERICAN PHYSICAL SOCIETY VIRTUAL JOURNAL OF BIOLOGICAL PHYSICS RE- SEARCH 6(2), (2003))

37. ***Molecular Dynamics Simulation of a Dipalmitoylphosphatidylcholine Bilayer with NaCl,***
Sagar A. Pandit, David Bostick, Max L. Berkowitz,
Biophys J, 84(6), 3743–3750, 2003.

38. ***Shape anisotropy and Voids***
Gauri R. Pradhan, Sagar A. Pandit, Anil D. Gangal, V. Sitaramam,
J Theor Biol, 220 (2), 189–199, 2003.

39. ***Molecular Dynamics Simulation of Dipalmitoylphosphatidylserine Bilayer with Na^+ counterions,***
Sagar A. Pandit, Max L. Berkowitz,
Biophys J, 82 1818–1827, 2002.

40. ***Random spread on the family of small-world networks,***
Sagar A. Pandit, R. E. Amritkar,
Phys Rev E, 63 1104, 2001.

41. ***Characterization of Small-world networks,***
Sagar A. Pandit, R. E. Amritkar,
Phys Rev E, 60 R1119, 1999.

42. ***Effect of doping on transport in 2-dimensional computational model for lipid biomembrane: Numeri- cal simulations reproducing experimental features,***
Gauri R. Pradhan, Sagar A. Pandit, Anil D. Gangal and V. Sitaramam,
Physica A, 270 288-294, 1999.
(ALSO APPEARS IN PHYSICS OF LIFE (ELSEVIER, INTERDISCIPLINARY WEB JOURNAL) http://www.elsevier.nl/locate/physoflife)

43. ***On generalized Nambu mechanics,***
Sagar A. Pandit, Anil D. Gangal,
J Phys: A, 31 2899, 1998.

Research Statement

My research focus is on theoretical/computational soft matter physics and biophysics. This work spans two research clusters identified by the School of Natural Sciences and Mathematics, viz. Computational Sciences and Bio-molecular systems. Hence, my work is broadly divided into two types:

1. Development of new simulation methods, and
2. Application of methods and techniques to biophysical problems.

Development of new simulation methods: Theoretical understanding of biological phenomena require modeling and simulations at varied length and time scales, e.g. typical chemical reactions occur at picosecond time scales and angstrom length scales. The consequent conformational changes that lead to interesting biology may occur at microsecond (six orders of magnitude) time scales and micrometer (four orders of magnitude) length scales. Hence, our major focus is to develop simulation methods that work at various scales and a consistent way of deriving these methods from one another. At the smallest scale we are developing methods to simulate reactive molecular systems and at the largest scales we are developing mean field theory based methods to obtain coarse grained information about the system of interest.

Simulations of reactive systems: The accuracy and speed of modern quantum chemistry (QC) methods allow the geometries, energies, and vibrational energies to be predicted quite accurately for small molecules. However, QC is not yet practical for studying the dynamic properties of larger molecules and solids. Consequently, it is useful to have accurate force fields (FF) to quickly evaluate forces and other dynamical properties such as the effects of mechanical shock waves, diffusion of small molecules, or structural properties of small biological molecules. However, in general, these force fields do not describe chemical reactivity. There are several modeling attempts to describe chemical reactions in terms of molecular mechanical force fields. We are developing computational methods for implementation of one such reactive force field proposed by van Duin et al (J. Am. Chem. Soc., 127, 11053 (2005)). This force field consists of a general bond-order-dependent potential in which the van der Waals and Coulomb forces are included from the beginning and the dissociation and reaction curves are derived from QC calculations. Efficient implementation of this force field requires sophisticated computational methods and algorithms. Currently, the code is publicly available as open software. A part of this code already appears in the popular open source software LAMMPS. Our implementation details are published in ***SIAM J. Sci. Comput., 34(1), C1–C23, 2012*** and ***Parallel Computing 38, 245–259, 2012***. As a first application of this method we have studied a Silica-water interface and investigated various modes of hydrogen transfer in Silica bulk (***J. Chem. Phys.,132, 174704, 2010***). In the future, this method will be used for simulation of proton transfer processes in biology and other important nano-material systems.

Database centric molecular dynamics simulation (DCMS): Molecular simulations have become an integral part of molecular and structural biology. The last couple of decades have seen tremendous development in computational systems for molecular simulations in both hardware and software aspects. At the present time, the field of simulations has many software systems employing their proprietary or open formats for data storage. The simulations by their nature generate large amount of data. Although many of the software systems are carefully designed to achieve maximum computational performance in the simulation tasks, they fall seriously short on storage and handling of the large scale data output. We have developed a

novel Database-centric Molecular Simulation (DCMS) framework that can connect to the high-efficiency computational power of existing molecular simulation software systems and augment it with the strong points of database systems for data storage and analysis. Such merging of these two technologies is producing a high throughput technique for simulations.
Some of the objectives of this project are to use database technologies to improve the efficiency, ease of maintenance, and security of molecular simulation data analysis. To this end we have already implemented a large scale database system under Postgres SQL and developed novel algorithms for analysis of large molecular trajectories. Our efforts on development of algorithms for computation of N-body correlation functions has resulted in extremely efficient algorithms that are part of the DCMS system (***IEEE Transactions on Knowledge and Data Engineering, 2012,*** and ***Proceedings of the 25th IEEE Intl Conference on Data Engineering, 2009***). These implementations are publicly available as open source software. Recently these algorithms have also been ported to GPU based systems and are currently under testing.

Self-consistent Mean field theory (SCMFT): I have developed a dynamical statistical mechanical model for lipid-cholesterol mixtures. My aim was to model lipid-cholesterol interactions in terms of the self-consistent, dynamical evolution of localized lipid molecular order parameters. Cholesterol molecules, within this model, were represented as small hard rods which interact with neighboring lipid chains to locally increase lipid chain order. The Hamiltonian is expressed in terms of the order parameters and the cholesterol position.
The Free Energy is calculated using the self--consistent mean field theory and the motion of the rods is driven by Langevin stochastic equations for center-of-mass and orientation of each cholesterol molecule. Unlike previous mesoscopic modeling attempts, coupling parameters in this model are obtained from molecular dynamics trajectories. The model is highlysuccessful in getting results that are consistent with new experimental findings (***Phys Rev E 83, 031925, 2011, J. Chem. Phys.,132, 174704, 2010,*** and ***Langmuir 24, 6858–6865 2008***).

Force Field optimization tools (FFOpt): The problem of parameter estimation in molecular dynamics corresponds to a highly non-linear optimization problem in a very high dimensional space. Given a set of training geometries, the optimization problem is to identify a set of force-field parameters such that the associated atomistic model (using our ReaxFF realization) yields the same physical properties as the quantum mechanically derived or experimentally observed (if available) training structures. Each molecular fragment in the training set is typically small (tens of atoms) and the resulting optimization problem is often under-constrained – i.e., a large number of force-field parameterizations are likely to yield geometries within specified tolerances. The problem is complicated by the fact that we need a single parametrization of the force-field that simultaneously optimizes all geometries in the training set.
The fitness of the parametrization for the input geometry is computed as the distance between the equilibrated atomistic-model generated geometry and the reference/training geometry. While the process of exploring this space is embarrassingly parallel, its computational cost necessitates development of novel optimization strategies that guide search to desirable parts of the parameter space. This is a formidable technical challenge. We have developed a novel approach and associated software system based on a modification of *Nelder-Mead* simplex optimization algorithm. The software is publicly available as an open source software and is being used by Dr. Chiu along with my students to develop simpler coarse-grain water force field parameters.

Applications to biophysics:

Lateral organization in membrane systems: Atomistic and Mean field simulations: There is abundant evidence that lateral inhomogeneities in composition and physical properties exist in biological membranes. These membrane lipid inhomogeneities play important roles in processes such as signal transduction and membrane traffic. In particular, there is a major focus on nano size membrane fragments which are not solubilized by the detergent Triton X-100. These domains are called detergent resistant membrane domains (DRM) or ``rafts''. At lower temperatures much of the sphingolipid and cholesterol components of mammalian cell membranes can be isolated in DRM fragments. It is well known that the extracted DRM domains are in a liquid ordered phase (Lo) in which lipid chains are highly ordered but whole lipid molecules have rotational and lateral diffusion coefficients comparable to those in the liquid crystalline (Lα) phase. The exact nature and the pathways involved in the lateral organization of membrane systems are still unknown. Such a lateral organization in the lipid membrane, which is due to the heterogeneity of the membrane constituents like various lipids, sterols, and transmembrane proteins, is believed to be spontaneous in many cases. My studies are aimed at understanding spontaneous organization in membranes, and involve molecular dynamics simulation and development of new mean field type coarse grain models (***J. Phys. Chem B, 116, 4500-4509, 2012, Phys Rev E 83, 031925, 2011, J. Chem. Phys.,132, 174704, 2010,*** and ***Langmuir 24, 6858–6865 2008***).

Modeling collagen molecules as short chain polymers: Molecular-dynamics simulations are performed on a model collagen molecule in SPC water, with and without 100 mM NaCl. To calculate the persistence length, we find the center of mass of each amino acid. We then group the amino acids into triplets, representing each by the (unweighted) average of the three centers of mass. These center-of-mass positions are used as end points for directors. The time-averaged cosine between directors is found (by determining the scalar product of the directors) as a function of contour length between them. Additionally, two-dimensional projections of the three-dimensional images are constructed, in analogy to the experimental deposition of collagen onto a surface. Techniques for measuring and calculating persistence length from AFM images are used on the two-dimensional projection images, and results are compared to the model prediction and to actual experimental results

Oxidative damage to lipid bilayer: Current simulations of lipid bilayers focus on their structural and compositional properties. Chemical reactivity between cell membranes and extra cellular species is an unexplored field for molecular dynamics. To explore this new area of research, we have simulated a lipid bilayer composed of 200 POPC lipids (along with 50 waters per lipid) and its reaction with a simple peroxide for 8 ns using Reactive Molecular Dynamics. The specific chemical pathways of oxidative damage can be determined from these simulations and a greater insight into the process can be achieved.

Teaching Statement

Educating the next generation of bright young minds is an essential aspect of my chosen career. Shaping the future in this manner is an especially fulfilling aspect of academic life.

In my opinion graduate and undergraduate science education must focus on three primary goals,

1. Imparting knowledge of well understood scientific theories and reality, as understood at the present time,
2. Development of independent and critical thinking, and
3. Development of practical tools and techniques for future academic and non--academic careers.

Achievement of each of these goals requires an instructor to adopt different types of teaching methods. In my opinion, student interaction within and outside the classroom is absolutely essential in fulfilling these objectives. To this end, I usually employ the approach of “directed discovery” in my classroom with emphasis on one-on-one meetings outside the class, during office hours. Whenever possible, I insist on assigning short-term class projects or possibly long-term research projects in my lab. This approach prepares students with technical know-how that can become a corner stone in their future endeavors.

In my classroom teaching, I have often observed that students have preconceived notions of the physical reality that surrounds them. These preconceptions may not always be well-founded. However, students rarely confront themselves about the correctness/validity of their understanding of physical reality. In the course of my undergraduate and graduate teaching I have tried to approach this goal of “imparting knowledge of well understood scientific theories” in three steps

1. I examine the physical processes and associated theories in class to identify possible misconceptions that may arise.
2. I construct a number of examples and more importantly counter examples to illustrate these ideas. Further, I assign several problems that focus on counterintuitive aspects of the physical theory. In smaller classrooms this approached has indeed helped students understand the basics of physical theories. Unfortunately for a large class, without TA support, it is harder to evaluate several homework assignments and provide fruitful feedback to a student. I have tried to fill this gap by making my lecture notes and solutions electronically available to the students through the “Blackboard system”.
3. I use every opportunity to revisit steps a. and b. during discussions outside the classroom.

To develop independent and critical thinking I have tried the approach of “guided discovery”. In this approach I pose a question/problem in the class and solicit student response to develop a scientific theory or solution of the posed problem. Usually, as a rule, I require the students to work individually or in small groups to solve different aspects/stages of the problem. For tangential thinkers, required clues or redirections are provided in the class, as well as through carefully designed homework assignments and quizzes. This method forces students to think independently and also makes them confident of their role in the discovery process. The approach was specifically very successful in my undergraduate introduction to quantum mechanics class (PHY 4604). In this course I stated (hammered in) the postulates of quantum mechanics (within the Copenhagen interpretation) at the beginning of the course and derived the entire quantum framework using the directed discovery approach. The approach was also

successful in my graduate computational physics class (PHZ 5156C). However, in large class courses such as PHY 2048, the approach worked with only a limited number of students who invested efforts outside the class or enrolled for the problem solving class PHY 2021 with me.

To develop technical knowledge I assign carefully chosen project topics at the beginning of the course. These projects are related to the course material but they rely on the development/study of particular numerical/mathematical/programming techniques that are usually outside the scope of the course. To cite a few examples, one such project assigned in my computational physics course (PHZ 5156C) was the study, implementation, and comparison of the symplectic integration algorithm with the other simple integrators such as Runge--Kutta. By the end of the semester, the concerned student had studied slightly advanced concepts in mathematics as well as some aspects of MATLAB and C programming, which I believe would be useful in their careers. In PHY 4604 a challenge was proposed, for extra credit, in class to solve a quantum mechanical problem using perturbation expansion as well as numerically on the computer (numerical solution was outside the defined scope of the course).

Apart from classroom teaching, I have served as a research mentor for undergraduate and high-school students in my group. In my opinion, exposure to research environment prepares these students in their studies and career.

New courses designed

I taught **8** different courses in last **5** years at USF. I completely redesigned the following **2** courses.

PHZ 5156C : Graduate Computational Physics:
This advanced level course is designed for graduate students with previous training in computational methods. I specifically chose topics on new programing paradigms and techniques.

The course had two main sections:
1. The basics: involved advanced topics like how code executes, performance issues, writing and profiling code. Frequently used data structures and codes, good programming practice. Parallel programming: paradigm shift , interprocess communication, various parallelization models, threads, messages, MPI.
2. Four aspects of computational physics: evaluation, solution, simulation, and data modeling.

The course evaluations were 4.20/5.0. Most students seem to enjoy and use the course material later in their research. In that respect the course was successful.

PHY 5937, PHZ 4151C : Undergraduate Computational Physics:
The course goal is to familiarize students with the use of computers in solving problems in physics and various science and engineering fields. The students are expected to be conversant with General Physics I, II, a year of calculus and Modern Physics. The course does not assume any background in programming.

The course was taught using the programming language “C”. The “C” programming language forms the basis for learning many similar compiled languages. Knowledge of such compiled

languages is expected to make the students more desirable in academia as well as the software or information technology industries. The course had three sections:

1. The language: learning the “C” language.
2. Computer solutions of mathematical problems in science and engineering: students learn to solve ordinary differential equations and partial differential equations on computers. Of course they studied a substantial amount of numerical linear algebra in the process.
3. Computer solutions of non-mathematical problems in science and engineering: students learn various simulation techniques including agent based modeling, cellular automaton etc.

The most challenging part of the course was teaching the “C” programming language in four weeks. This was achieved by first introducing a subset of the language that can be described as purely functional (in the sense of a functional language, even though internally it is not) and then introduce the primitive “side effects” (such as pointers and objects) through examples.

So far I have taught the course twice. Most students performed reasonably well but the ones who did not performed well seem to have problems with mathematical thinking. I am working on developing new examples that are less mathematical. Overall the course was successful as a few students got hired in software industry after the course.