

# SHANTANU SHARMA CURRICULUM VITÆ

Department of Biochemistry & Biophysics  
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## RESEARCH INTERESTS

Biophysics, computational biology, systems biology, data mining.

## EDUCATION

### **Ph.D. Biochemistry.** *University of North Carolina, Chapel Hill, 2009*

Dissertation: Computational modeling and automation techniques to study biomolecular dynamics.

Advisor: Prof. Nikolay V. Dokholyan

Graduate emphasis in *Bioinformatics & Computational Biology*.

Graduate emphasis in *Molecular & Cellular Biophysics*.

### **B.Tech. Computer Science & Engineering.** *Indian Institute of Technology, Kanpur, 2004*

Dissertation: A novel approach to structural comparison of proteins.

Advisor: Prof. Somenath Biswas

Graduate coursework in *Bioinformatics & Molecular Biology*.

## HONORS AND AWARDS

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|-----------|--|
| 2008      | TeraGrid Resource Award for Multiscale Simulations of Biomolecular Dynamics.   |
| 2007–2009 | NIH Integrated Biomedical Research Training Program (IBRTP) Fellowship.  |
| 2004–2009 | Full scholarship and tuition waiver for doctoral research.   |
| 2008      | Awarded postdoctoral fellowship at Vanderbilt University based on doctoral research.   |
| 2007      | National Biomedical Computation Resource Summer Fellowship.  |
| 2007      | Apple Worldwide Software Developers Conference Scholarship 2007 (WWDC07), Apple Inc.   |
| 2007      | American Society for Biochemistry and Molecular Biology Travel Fellowship to present doctoral research at the Experimental Biology 2007, ASBMB Annual Meeting 2007.  |
| 2007      | American Association for the Advancement of Science, Nominated Membership to Program for Excellence in Science.  |
| 2004–2006 | NIH Molecular & Cellular Biophysics Graduate Research Fellowship.  |
| 2003–2004 | Award equivalent to \$10,000 by Annual Class of 1976 IIT Kanpur Alumni Funds Competition for research towards a microcontroller-based prepayment energy meter.   |
| 2003–2004 | BioGeometry Project Undergraduate Research Award (\$10,000), mentored by Dr. CW Carter Jr., Dr. JM Roach, Biochemistry & Biophysics, University of North Carolina.   |
| 2004      | Honorarium equivalent to \$1,000 by Indian Institute of Technology Kanpur for lecturing in IIT Kanpur Data Structures and Algorithms Summer School 2004.   |
| 2000      | Gold Medal in Indian National Physics Olympiad 2000, awarded to top 30 students from >30,000 candidates in India. Attended the International Physics Olympiad Camp, Homi Bhabha Center for Science Education, Mumbai, India.                 |
| 2000      | Silver Medal and fellowship equivalent to \$4,000 for securing 64 <sup>th</sup> rank (among 1,50,000 candidates) in Indian Institutes of Technology Joint Entrance Examination 2000, FIITJEE Ltd, New Delhi and Apex Academy, Mumbai, India. |

- 2000 Fellowship equivalent to \$1,000 for securing 5<sup>th</sup> rank (among 1,50,000 candidates) in MP State Level Pre-Engineering Test 2000, Professional Examination Board, Bhopal, India.
- 2000 Awarded Certificate of Merit for outstanding performance in the Indian National Chemistry Olympiad 2000 by the Homi Bhabha Centre for Science Education, Tata Institute of Fundamental Research, Mumbai, India.
- 1998 Fellowship equivalent to \$1,000 for securing first merit rank (among >50,000 candidates) in State-Level Senior Science Competition, MP Council of Science & Technology, Bhopal, India.
- 1998–2004 Indian National Talent Search Scholarship; Awarded to top 1% of 50,000 candidates by National Council for Educational Research & Training, New Delhi, India.
- 1998–2000 Awarded Merit Certificate by the Central Board of Secondary Education for outstanding academic performance (top 0.1%) in Mathematics (10th grade, 1998), Physics (12th grade, 2000).
- 1998–1999 Awarded Merit Certificate for meritorious performance in the National Mathematics Olympiad Contest by the Delhi Association of Mathematics Teachers at junior (1998) and intermediate (1999) levels.

### REFEREED JOURNAL PUBLICATIONS

1. **Shantanu Sharma**, Lisa Vogel, Brian D Strahl, and Nikolay V Dokholyan. "High resolution discrete molecular dynamics simulations of yeast nucleosome reveal residues that contribute to nucleosome stability." *Biophysical Journal* (2009). Submitted.
2. **Shantanu Sharma**, Feng Ding, and Nikolay V Dokholyan. "iFoldRNA: three-dimensional RNA structure prediction and folding." *Bioinformatics* **24**, 1951–1952 (2008). Journal Impact Factor: 6.1, Citations: 1.
3. Feng Ding, **Shantanu Sharma**, Poornima Chalasani, Vadim V Demidov, Natalia E Broude, and Nikolay V Dokholyan. "Ab initio RNA folding by discrete molecular dynamics: From structure prediction to folding mechanisms." *RNA* **14**, 1164–1173 (2008). Journal Impact Factor: 5.8, Citations: 4.
4. **Shantanu Sharma**, Feng Ding, and Nikolay V Dokholyan. "Probing protein aggregation using simplified models and discrete molecular dynamics." *Frontiers in Biosciences* **13**, 4795–4808 (2008). Journal Impact Factor: 3.6, Citations: 1.
5. **Shantanu Sharma** and Nikolay V Dokholyan. "DNA sequence mediates nucleosome structure and stability." *Biophysical Journal* **94**, 1–3 (2008). Journal Impact Factor: 4.8, Citations: 1.
6. **Shantanu Sharma**, Peng Gong, Brenda Temple, Debadeep Bhattacharyya, Nikolay V Dokholyan, and Stephen G Chaney. "Molecular dynamic simulations of cisplatin- and oxaliplatin-d(GG) intrastand cross-links reveal differences in their conformational dynamics." *Journal of Molecular Biology* **373**, 1123–1140 (2007). Journal Impact Factor: 4.5, Citations: 8.
7. **Shantanu Sharma**, Yiwen Chen, Feng Ding, Huifen Nie, Adrian W Serohijos, Kyle C Wilcox, Shuangye Yin, and Nikolay V Dokholyan. "Protein folding: Then and now." *Archives of Biochemistry and Biophysics* **469**, 4–19 (2008). Journal Impact Factor: 2.6, Citations: 7.
8. **Shantanu Sharma**, Feng Ding, and Nikolay V Dokholyan. "Multiscale modeling of nucleosome dynamics." *Biophysical Journal* **92**, 1457–1470 (2007). Journal Impact Factor: 4.8, Citations: 28.
9. **Shantanu Sharma**, Feng Ding, Huifen Nie, Daniel Watson, Aditya Unnithan, Jameson Lopp, Diane Pozefsky, and Nikolay V Dokholyan. "iFold: a platform for interactive folding simulations of proteins." *Bioinformatics* **22**, 2693–2694 (2006). Journal Impact Factor: 6.1, Citations: 10.
10. Kerry Bloom, **Shantanu Sharma**, and Nikolay V Dokholyan. "The path of DNA in the kinetochore." *Current Biology* **16**, 276–278 (2006). Journal Impact Factor: 11.7, Citations: 21.
11. Jeffrey Roach, **Shantanu Sharma**, Maryna Kapustina, and Charles W Jr Carter. "Structure alignment via Delaunay tetrahedralization." *Proteins Structure, Function and Bioinformatics* **60**, 66–81 (2005). Journal Impact Factor: 4.7, Citations: 16.

REFEREED CONFERENCE ARTICLES

12. **Shantanu Sharma**, Vinay Choudhary, and Ratan K Ghosh. "AAB: A generalized java-based algorithm animator builder." *In Proceedings of the Fifth International Conference of Information Technology* (Tata McGraw Hill, 2002).

BOOK CHAPTERS

13. Jessica McCann, **Shantanu Sharma**, and Justin Brown. *Best Practices In Biotechnology Education*, chapter Carolina Student Biotechnology Network (ThinkBiotech, 2008).
14. Stephen G Chaney, Srinivas Ramachandran, **Shantanu Sharma**, Nikolay V Dokholyan, Brenda Temple, Debadeep Bhattacharyya, Yibing Wu, and Sharon Campbell. *Platinum and Other Heavy Metal Compounds in Cancer Chemotherapy*, chapter Differences in conformation and conformational dynamics between cisplatin and oxaliplatin DNA adducts (Springer, 2009).

TECHNICAL REPORTS

15. **Shantanu Sharma** and Somenath Biswas. "A novel approach to structural comparison of proteins." Technical Report, Department of Computer Science and Engineering, Indian Institute of Technology Kanpur (2004).
16. **Shantanu Sharma** and Nitin K Dahra. "PVM, MPI and OpenMP: A comparison and suitability for various architectures." Technical Report, Department of Computer Science and Engineering, Indian Institute of Technology Kanpur (2004).
17. **Shantanu Sharma** and Nimit Kumar. "Independent component analysis of real and complex Fourier space: an application to videos and natural scenes." Technical Report, Department of Computer Science and Engineering, Indian Institute of Technology Kanpur (2004).
18. **Shantanu Sharma**, Nitin Gupta, and Amitabha Mukherjee. "An active appearance model based face-recognition system." Technical Report, Department of Computer Science and Engineering, Indian Institute of Technology Kanpur (2003).
19. **Shantanu Sharma** and Mathad S Apurva. "Neural network applications in sensor fusion." Technical Report, Department of Computer Science and Engineering, Indian Institute of Technology Kanpur (2003).

ABSTRACTS (INVITED & CONTRIBUTED)

20. **Shantanu Sharma** and Nikolay V Dokholyan. "Exploring core histone residues mediating chromatin stability." 2008 Annual UNC Biophysics Graduate Research Forum, Chapel Hill, NC, USA (2008). Invited Talk.
21. **Shantanu Sharma** and Nikolay V Dokholyan. "Engineering site-directed mutagenesis in nucleosomes to probe in vivo chromatin stability." Institute of Biological Engineering Annual Conference 2008, Chapel Hill, NC, USA (2008). Invited Talk.
22. **Shantanu Sharma** and Nikolay V Dokholyan. "Understanding chromatin dynamics - modeling and rational design." UNC Bioinformatics and Computational Biology Colloquium, Chapel Hill, NC, USA (2008). Invited Talk.
23. **Shantanu Sharma**, Lisa Vogel, Brian Strahl, and Nikolay V Dokholyan. "Role of Conserved Histone Core in Nucleosome Stability." 2nd Annual Atlantic Coast Chromatin Conference 2007, Chapel Hill, NC, USA (2007). Poster Presentation.
24. **Shantanu Sharma** and Nikolay V Dokholyan. "Structural organization and dynamics of the kinetochore." 2nd Annual Duke Systems Biology Symposium 2007, Durham, NC, USA (2007). Poster Presentation.
25. **Shantanu Sharma**. "Modeling chromatin structure and dynamics." 2007 UNC Biochemistry and Biophysics Summer Seminar Series, Chapel Hill, NC, USA (2007). Invited Talk.

26. **Shantanu Sharma**. “Simulations probing mechanisms of Platinum anticancer drugs.” 2007 UNC Molecular and Cellular Biophysics Forum, Chapel Hill, NC, USA (2007). Invited Talk.
27. **Shantanu Sharma** and Nikolay V Dokholyan. “Investigating protein dynamics using multiscale simulations.” 2007 Annual UNC Biochemistry and Biophysics Research Retreat, Chapel Hill, NC, USA (2007). Poster Presentation.
28. **Shantanu Sharma** and Nikolay V Dokholyan. “iFold – web-based multiscale modeling of protein dynamics.” 2007 Annual UNC Bioinformatics and Computational Biology Research Seminar, Chapel Hill, NC, USA (2007). Poster Presentation.
29. **Shantanu Sharma**. “The odyssey of chromatin organization – histone tails and variants.” 2007 North Carolina Theoretical and Systems Biology Seminar Series, Chapel Hill, NC, USA (2006). Invited Talk.
30. **Shantanu Sharma** and Nikolay V Dokholyan. “Integrating multiscale modeling and simulations with scalable high performance computation.” 2007 Annual Symposium on Cyberinfrastructure and Multiscale Modeling Approaches, 2007, San Diego, CA, USA (2007). Poster Presentation.
31. **Shantanu Sharma** and Nikolay V Dokholyan. “Nucleosome dynamics in silico – role of DNA and histone tails.” 98th Annual Meeting of the American Society for Biochemistry and Molecular Biology, Washington, DC, USA (2007). Poster Presentation.
32. Debadeep Bhattacharya, Candice King, **Shantanu Sharma**, Brenda Temple, Sharon Campbell, and Stephen G Chaney. “Effect of sequence context in platinum–DNA structure.” 98th Annual Meeting of the American Association for Cancer Research, Los Angeles, CA, USA (2007). Poster Presentation.
33. **Shantanu Sharma**, Feng Ding, and Nikolay V Dokholyan. “Discrete molecular dynamics studies of nucleosomes.” 51st Annual Meeting of the Biophysical Society, Baltimore, MD, USA (2007). Platform Presentation.
34. **Shantanu Sharma** and Nikolay V Dokholyan. “Histone variants and tail dynamics in chromatin organization.” 6th Biennial Carolina Biophysics Symposium 2006, Chapel Hill, NC, USA (2006). Poster Presentation.
35. **Shantanu Sharma** and Nikolay V Dokholyan. “Structural dynamics of a nucleosome.” 1st Annual Duke Systems Biology Symposium 2006, Durham, NC, USA (2006). Poster Presentation.
36. **Shantanu Sharma**, Kerry Bloom, and Nikolay V Dokholyan. “Structure and dynamics of centromere specific nucleosomes.” 1st Annual Atlantic Coast Chromatin Conference 2006, Chapel Hill, NC, USA (2006). Poster Presentation.
37. Tamara James, **Shantanu Sharma**, and Nikolay V Dokholyan. “Comparing unfolding and folding pathways for Eglin C, SH3, and Chymotrypsin Inhibitor-2.” 2005 Annual Meeting of the HHMI UNC Partnership for Minority Students in Biomolecular Sciences 2005, Chapel Hill, NC, USA (2005). Poster Presentation.
38. Aram Kim, **Shantanu Sharma**, Jeffrey Roach, and Charles W Carter. “Multiple sequence and structure alignments.” International Conference on Aminoacyl-tRNA Synthetases: Ancient Molecules for Future Biology and Medicine, Seoul, South Korea (2004). Poster Presentation.

#### MEDIA COVERAGE

39. “Playing hard balls with RNA: fully automated ab initio RNA folding by discrete molecular dynamics.” Drug Discovery Today (2008).
40. “ITS supports iFold protein folding endeavor.” University of North Carolina ITS In Review (2006).

RESEARCH GRANT-WRITING EXPERIENCE

- ◊ National Institutes of Health grant on Project iFold (2007) – high priority score.
- ◊ North Carolina Biotechnology Center grant on chromatin research (2006) – funded in full.
- ◊ National Institutes of Health grant on modeling chromatin dynamics (2006) – high priority score.
- ◊ National Institutes of Health grant on computer architectures for simulations – high priority score.

TEACHING RECORD

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|------------|--|
| 5–5/2007   | Invited Lecturer, Biochemistry Comprehensive Examination Study Group. Class of 20 graduate students, Department of Biochemistry & Biophysics, UNC Chapel Hill.                 |
| 2–2/2007   | Invited Lecturer, Integrated Biomedical Research Seminar Class of 40 undergraduate students, Department of Biology, UNC Chapel Hill.   |
| 9–11/2005  | Teaching Assistant, Macromolecular Structure and Dynamics Class of 20 graduate students, Department of Biochemistry & Biophysics, UNC Chapel Hill.                             |
| 4–7/2004   | Course Instructor, Summer Course in Algorithms and Data Structures, Class of 60 undergraduate and graduate students, Department of Computer Science & Engineering, IIT Kanpur. |
| 10–10/2003 | Lecturer, Lectures on Scientific Computing using Linux, Class of 100 Undergraduate/Graduate Students, Department of Computer Science & Engineering, IIT Kanpur.                |

STUDENTS COLLABORATED AND MENTORED

- |           |  |
|-----------|--|
| 2007–2009 | Sunny Darji, Undergraduate Research Intern, Department of Biochemistry, UNC Chapel Hill.   |
| 2007–2009 | Lisa Vogel, Undergraduate Research Intern, Department of Chemistry, UNC Chapel Hill.   |
| 2007–2008 | Adrian Randall, Undergraduate Research Intern, Department of Chemistry, UNC Chapel Hill.   |
| 2006–2007 | Tamara J. James, Bachelor of Science Thesis, Senior Year Research, Department of Natural Sciences, Johnson C. Smith University.                    |
| 2005–2006 | Daniel Watson, Aditya Unnithan, Jameson Lopp, Undergraduate Software Engineering Project, Department of Computer Science, UNC Chapel Hill.         |
| 2001–2004 | Vivek Mishra, Akshat Jain, Har Kishore Rai, Sharad Shrivastava, Sai Pritham, Zulfikar Ali, Mentored under Students' Counseling Program, IIT Kanpur |

PROFESSIONAL EXPERIENCE

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|-----------|---|
| 2008–2009 | <b>Technology Transfer Intern</b> at <i>University of North Carolina Office of Technology Development</i> , Chapel Hill, NC, USA. Professional experience in technology transfer, patent processing and market research analytics.  |
| 2004–2009 | <b>Graduate Research Assistant</b> at <i>Dokholyan Research Group</i> , UNC Chapel Hill, NC, USA. Research & development to simulate and analyze chromatin dynamics at unprecedented detail. Collaborated with many interdisciplinary teams on multidisciplinary research projects ( <i>cf.</i> Publications). Designed iFold, a scalable web-based molecular simulation portal (Grid middleware, Java, C, php, Perl). Designed the first RNA folding tool with web front-end and a 4000 node Linux cluster backend (Java, C). Administered the computational laboratory with 1 TB NAS, Gigabit network and >15 Linux workstations. |
| 2006–2007 | <b>Student Developer</b> at <i>Apple Inc.</i> , (Offsite) Cupertino, CA. Developed research analytical tools using C++ and XCode. Awarded Apple Worldwide Student Scholarship to attend Apple Worldwide Developers Conference 2007.   |
| 2007–2007 | <b>Research Intern</b> at <i>National Biomedical Computation Resource</i> , San Diego, CA. Research in cyber-infrastructure, grid/cluster computing and multiscale modeling.  |

- 2004–2004 **Instructor** at *Summer Course in Algorithms and Data Structures*, IIT Kanpur, India. Lectured algorithms, data structures to a class of >50 graduate and undergraduate students. Designed and evaluated examinations in algorithm design and data structure modeling.
- 2003–2004 **Undergraduate Research Fellow** at *BioGeometry Project*, Chapel Hill, NC, USA. Developed a tool for rapid protein structure comparison using Delaunay tessellation (C, C++).
- 2002–2003 **Bioinformatics Research Scholar** at *National Center for Biological Sciences*, Bangalore, India. Developed SBL++, an efficient object-oriented class library for structural bioinformatics (C++).
- 2002–2002 **Computational Research Intern** at *Computational Mathematics Laboratory, Tata Institute*, Pune, India. Research in improving the existing Karmarkar's algorithm for 3SAT boolean satisfiability problem by reducing duality gap and analysis of symmetric Gaussian matrices.

## SKILL SUMMARY

- ◇ **Programming Languages:** *Proficient in C, C++, Java, & Shell Scripting. Fluent in SQL, Python, MATLAB, Perl & Fortran. Familiar with R, Oracle, Lisp, ML, JavaScript, & 8086 Assembly.*
- ◇ **Bioinformatics:** Insight-II, Sybyl, Spock, BLAST, PyMol, VMD, Gromacs, Amber, Rasmol, & Kinemage.
- ◇ **Applications:** Lex, Yacc/Bison, Adobe Photoshop, Adobe Illustrator, & MS Access.
- ◇ **Technologies:** XML, HTML/CSS, GTK, CVS, SVN & QT.
- ◇ **Operating Systems:** Linux, Windows, Mac OS X, AIX, Solaris, & HP-UX.

## SIGNIFICANT SOFTWARE PROJECTS

- ◇ TuXilla: A multithreaded FTP download client for Linux having a graphical user interface (C, Socket API).
- ◇ Active Appearance Model based face recognition system (Sponsored by Adobe, India) (C++, Java).
- ◇ SmartMeter: A design for microcontroller based solid-state prepayment energy meter (C++).
- ◇ Extended Nachos: virtual memory, system calls, synchronization, scheduling, multi-tasking (C).
- ◇ Hades: An application for streaming distributed multimedia resources over a local area network (C, Gtk).
- ◇ Algorithms and implementation of the Chinese checkers game strategy using alpha-beta pruning (Java).
- ◇ Independent component analysis in complex Fourier space: spatiotemporal dynamics of videos (MATLAB).

## TEAM LEADERSHIP AND COMMUNITY SERVICES

- 2008 Relief work and fund-raising for flood victims in Indian villages.
- 2007 Chair, Platform session on Chromatin, 51<sup>st</sup> Annual Meeting of the Biophysical Society, Baltimore, MD, USA.
- 2008–Present Manuscript reviewer for *Molecular Systems Biology*.
- 2008–Present Manuscript reviewer for *Genome Biology*.
- 2007–Present Manuscript reviewer for *Journal of Chemical Theory and Computation*.
- 2006–Present Manuscript reviewer for *Journal of Molecular Biology*.
- 2006–Present Manuscript reviewer for *Biophysical Journal*.
- 2006–2008 Executive, Carolina Student Biotechnology Network, NC USA (<http://www.carolinabiotech.org>).
- 2006–2008 Member, Training Initiative in Biomedical and Biological Sciences, NC USA (<http://www.unctibbs.org>).
- 2003–2004 Head, Students Computing Services, IIT Kanpur, India (<http://students.iitk.ac.in/gymkhana>).

## SHANTANU SHARMA CURRICULUM VITÆ (7 of 7)

- 2002–2003 President, Association for Computing Activities, IIT Kanpur, India (<http://www.cse.iitk.ac.in/users/aca>).
- 2002–2003 Science & Technology Development Leader, IIT Kanpur, India (<http://students.iitk.ac.in/gymkhana>).
- 2002–2003 Coordinator, Public Relations Cell, Students' Gymkhana IIT Kanpur, India (<http://antaragni.iitk.ac.in>).
- 2001–2002 Students' Counselor, Undergraduate Counseling Service, IIT Kanpur, India (<http://www.iitk.ac.in/counsel>).
- 1999–2000 Head Boy, Delhi Public School, Bhilai, India (<http://www.dpsfamily.org>).
- 1998–1999 House Prefect, Jhelum, Delhi Public School, Bhilai, India (<http://www.dpsfamily.org>).

### ACADEMIC AND INDUSTRIAL AFFILIATIONS

- 2007–Present International Society for Computational Biology, La Jolla, CA USA (<http://www.iscb.org>).
- 2007–Present American Association for the Advancement of Science, Washington, DC USA (<http://www.aaas.org>).
- 2002–Present Association for Computing Machinery, New York, NY USA (<http://www.acm.org>).
- 2004–Present IIT Kanpur Alumni Association, IIT Kanpur, India (<http://www.iitkalumni.org>).
- 2006–2008 Biophysical Society, Bethesda, MD USA (<http://www.biophysics.org>).
- 2006–2008 American Chemical Society, Washington, DC USA (<http://www.acs.org>).
- 2006–2008 The Epigenetics Society, Gainesville, FL, USA (<http://www.dnamethsoc.com>).
- 2005–2007 Apple Developer Connection, Cupertino, CA USA (<http://www.apple.com>).

### REFERENCES

References are available upon request.