Tanmoy Sanyal

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Appointments

2019- **Postdoctoral scholar**, *Sali Lab*, Department of Bioengineering and Therapeutic Sciences, University of California San Francisco, CA, USA

Education

2013- 2018 **Ph.D**, *Chemical Engineering*, University of California Santa Barbara, CA, USA

2014- 2016 **Graduate emphasis**, *Computational Science and Engineering*, University of California Santa Barbara, CA, USA (Specialization in numerical methods for differential equations, and parallel computing)

2008- 2013 **Masters and Bachelors of Technology (Hons.) integrated dual degree**, *Chemical Engineering*, Indian Institute of Technology Kharagpur, WB, India

Research Interests

Integrative protein structure modeling using chemical crosslinking data, protein-protein docking, representation learning of protein graphs, probabilistic machine learning, coarse-graining of molecular dynamics simulations

Skills

Softwares MATLAB, Lammps, Gromacs, IMP, Modeller, VMD, UCSF Chimera/X

ML libraries PyTorch, Tensorflow, PyMC3

Languages Python (~10000+ lines), Fortran-90 (~1000+ lines), C++ (~2000+ lines), Bash, TCL

Research Experience

UCSF Postdoc advisor: Andrej Sali

- **Protein structure modeling using chemical crosslinks:**
  I develop computational protein structure models by integrating homology models with mass-spectrometry-chemical-crosslinking data. Beyond the traditional use as distance restraints in modeling, I employ crosslink data in new and innovative ways to learn domain representation and perform automatic fragment assembly in protein complexes. I use deep learning techniques to develop computationally fast yet thermodynamically accurate atomistic models of crosslinking peptides. Application of these methods include chromosomal maintenance (Smc5/6) and repair (DNA helicase) proteins. Recent projects also include computational epitope mapping of antibodies and nanobodies for host-pathogen systems.

- **Whole cell models:**
  As a part of the Pancreatic Beta-Cell Consortium (collaborating across UCSF, USC, SanghaiTech and HUJI), I use Bayesian networks to combine disparate models of the cell such as continuum scale pharmacokinetic models, particle scale Brownian Dynamics models and statistical network models of enzymatic pathways, to build an overarching *metamodel* of the cell.

UCSB PhD advisor: M. Scott Shell

Thesis: Next-Generation Coarse-Grained Models for Molecular Dynamics Simulations of Fluid Phase Equilibria and Protein Biophysics Using the Relative Entropy

- Introduced the local density potential for structurally and thermodynamically accurate coarse-grained molecular dynamics (MD) simulations of liquid-liquid phase separation, which are relatively rare in the chemical engineering literature.

- Developed protein backbone models for (a) template-free folding of 200+ residue coarse-grained protein domains using MD simulations and, (b) studying self-assembly in amyloidogenic peptides.

IIT Kharagpur Undergraduate thesis advisor: Saikat Chakraborty

Reactive-diffusive modeling of human respiration and its application in characterizing the patho-physiology of methemoglobin induced anemia (Awarded best bachelors thesis)

Computational experience

- **Generative models** - Experienced in parameterizing generative models, specifically variational autoencoders, using PyTorch.
- **Bayesian inference and Bayesian networks** - Experienced in building and sampling Bayesian networks for model selection, using PyMC3.
- **Analysis of high dimensional data** - Experienced in analyzing massively high-dimensional molecular dynamics trajectories to extract physically motivated low-dimensional projections and constructing meaningful visual representations.
- **High performance computing** - Parallelized runtime-critical parts of (PhD) group software using MPI. Also experienced in re-writing slow Python code as Fortran subroutines or Cython functions and wrapping back into Python as shared libraries.
- **Open-source contribution** - Code contributor to LAMMPS and the Integrated Modeling Platform (IMP).
- **Linux cluster management** - System administrator for (PhD) group Rocks 6.2 cluster. Installed Rocks and wrote post-install scripts to automate safe handling of the network-attached-storage and developed protocols to automate resource-sharing between lab members.

Publications

* authors have equal contribution

- F.D. Mast, P.C. Fridy, N.E. Karen, J. Wang, E.Y. Jacobs, J.P. Olivier, **T. Sanyal,** K.R. Molloy, F. Schmidt, M. Rutkowska, Y. Weisblum, L.M. Rich, E.R. Vanderwall, N. Dambrauskas, V. Vigdorovich, S. Keegan, J.B. Jiler, M.E. Stein, P.D.B Olinares, T. Hatziioannou, D.N. Sather, J.S. Debley, D. Fenyo, A. Sali, P.D. Bieniasz, J.D. Aitchison, B.T. Chait & M.P. Rout, *Highly synergistic combinations of nanobodies that target SARS-CoV-2 and are resistant to escape"*, (2021), eLife (*just accepted*, a preprint can be found at bioRxiv 2021.04.08.438911)

- B. Raveh*, L. Sun*, K.L. White*, **T. Sanyal***, J. Tempkin, D. Zheng, K.B. Pilla, J. Singla, C,Wang, J. Zhao, A. Li, N.A. Graham, C. Kesselman, R.C. Stevens & A. Sali, *Bayesian metamodeling of complex biological systems across varying representations*. P. Natl. Acad. Sci. USA. (2021) 118(35), e2104559118

- Y. Yu*, S. Li*, Z. Ser*, **T. Sanyal***, K. Choi, B. Wan, H.Kuang, A. Sali, A. Kentsis, D.J. Patel & X. Zhao, *Integrative analysis reveals unique structural and functional features of the Smc5/6 complex*. P. Natl. Acad. Sci. USA. (2021) 118(19), e2026844118

- **T. Sanyal**, J. Mittal & M.S. Shell, *A hybrid, bottom up, structurally-accurate, Gō-like coarse-grained protein model*. J. Chem. Phys. (2019) 151, 044111 (*Editor's pick article, 2019*)

- D. Rosenberger, **T. Sanyal**, M.S. Shell & N.F.A. van der Vegt, *Transferability of local density-assisted implicit solvation models for homogeneous fluid mixtures.* J. Chem. Theory Comput. (2019) 15, 2881-2895

- M.P. Howard, W.F. Reinhart, **T. Sanyal**, M.S. Shell, A. Nikoubashman & A.Z. Panagiotopoulos, *Evaporation-induced assembly of colloidal crystals.* J. Chem. Phys. (2018) 149(9)

- **T. Sanyal** & M.S. Shell, *Transferable coarse-grained models of liquid-liquid equilibrium using local density potentials optimized with the relative entropy.* J. Phys. Chem. B (2018) 122 (21), 5678-5693

- **T. Sanyal** & M.S. Shell, *Coarse-grained models using local-density potentials optimized with the relative entropy: Application to implicit solvation.* J. Chem. Phys. (2016) 145, 034109

- **T. Sanyal** & S. Chakraborty, *Multiscale analysis of hypoxemia in methemoglobin-anemia.* Math. Biosci. (2013) 241, 167-180

- **T. Sanyal** & S. Chakraborty, *Multiscale analysis of simultaneous uptake of two interacting gases in the human lungs and its application to methemoglobin anemia.* Comput. Chem. Engg. (2013) 59, 226-242

Conference Presentations

- BPS Annual Meeting; San Francisco, CA (Feb. 2022) **Talk**: *Rigid body assignment in integrative determination of protein complex structures*, **abstract accepted and attendance confirmed**

- AIChE Annual Meeting; Boston, MA (Nov. 2021) **Talk**: *Playing Bayesian jigsaw with PDB structures: Optimizing rigid body representations for integerative modeling of macromolecular complexes*, & **Poster** *Integrative modeling of the Smc-5/6 protein complex*

- PDB50: A special symposium celebrating the 50th anniversary of the Protein Data Bank; virtual (May. 2021) **Posters**: *Integrative modeling of the Smc5/6 complex & Playing Bayesian jigsaw with PDB structures: Optimizing rigid body representations for integrative modeling*

- USC Bridge Institute - Pancreatic Beta Cell Consortium Retreat; Catalina Island, CA (Nov. 2019) **Workshop**: *Meta-modeling: Probabilistic graphical models and your data*

- Berkeley Mini Stat Mech Meeting; Berkeley, CA (Jan. 2019) **Poster**: *Coarse-grained models for protein folding and self-assembly with the relative entropy*

- 10^{th} Annual Amgen Clorox Graduate Student Symposium; UC Santa Barbara, CA (Oct. 2017) **Talk**: *A new approach to computationally fast coarse-grained models of hydrophobic interactions in fluids*

- AIChE Annual Meeting; San Francisco, CA (Nov. 2016) **Talk**: *Improved coarse-grained models through local density potentials, optimized with the relative entropy*

- Berkeley Mini Stat Mech Meeting; Berkeley, CA (Jan. 2015) **Poster**: *Building coarse grained models of solvation using local density dependent interactions with the relative entropy*

- Southern California Simulations in Science Conference; UC Santa Barbara, CA (Oct. 2015) **Poster**: *Building coarse grained models of solvation using local density dependent interactions with the relative entropy*

- 8^{th}Amgen-Clorox Graduate Student Symposium; UC anta Barbara, CA (Sept. 2015) **Poster**: *Robust models of coarse-grained interactions using multi-body potentials with the relative entropy*

- AIChE Annual Meeting; San Francisco, CA (Nov. 2013) **Poster**: *Stability of mixing limited patterns in isothermal homogenous autocatalytic reactions*

Teaching Assistance

Undergraduate Thermodynamics (Fall 2018), Undergraduate Reaction Engineering (Spring 2017), Graduate Thermodynamics (Fall 2015), Introduction to Chemical Engineering(Fall 2014

Relevant Courses

Thermodynamics, Equilibrium and Non-equilibrium statistical mechanics, Finite-Difference and Finite-Element methods for PDEs, Parallel computing

Awards

2012 Best bachelors thesis, IIT Kharagpur

2009 Technopreneur Promotion Programme, Ministry of Science and Technology, Govt. of India - seed money for prototype scale-up of novel bio-reactors for algal bio-diesel generation

2009 Jagdis Bose National Science Talent Search (JBNSTS) foundation, WB, India - fellowship

Volunteering

2021- Independent reviewer for Structure

2021- Member of eLife early-career reviewer pool

2014-2016 **Co-founder and co-organizer, ChE Graduate Simulation Seminar Series**

- Conceptualized and started a seminar series with colleagues to address the unfulfilled need for a common collaborative and social platform for theory and computation researchers on campus.
- Developed extensive public outreach and attracted funding from ChE, Materials and Computer Science faculty, with participation from over 10 STEM fields and special attendances and keynotes from industry and national labs