Tanmoy Sanyal

Scientist, Computational drug design & Structural biology

About

Greater Seattle area, WA

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tanmoy7989

Molecular modeling

Rosetta
openMM
LAMMPS
GROMACS
IMP
Modeller
UCSF ChimeraX
PyMOL
VMD

ML frameworks

PyTorch
Tensorflow
Tensorflow-probability
PyMC3

Workflows

Snakemake
AWS Batch

Languages

Python (+Cython) (~20000+ lines)
Fortran-90 (~1000+ lines)
C++ (~4000+ lines)
Bash
TCL

Open Source

LAMMPS
Local density potential

nbspike
Integrative epitope prediction

IMP
Crosslink guided domain discovery

PDB-Dev deposition
Structure of SMC5/6

Education

University of California Santa Barbara
2013 - 2018

Santa Babara, CA, USA

Ph.D Chemical Engineering

Graduate emphasis in Computational Science & Engineering (Parallel Computing & Numerical methods for ODEs / PDEs)

Indian Institute of Technology Kharagpur
2008 - 2013

Kharagpur, WB, India

Masters and Bachelors of Technology (Hons.) integrated dual degree Chemical Engineering

Research Experience

Novo Nordisk Research Center Seattle
2022 - Present

Scientist, Computational drug discovery

- **Biologics Design**: Design of peptides and antibodies for rare endocrine disorders, and SAR (structure activity relationship) analysis based on PLMs (protein language models)
- **Scientific Software development**: Computational workflows for automating molecular model building and MD simulation of modified peptides, such as small molecule acylations or peptide-biopolymer conjugates.

Department of Bioengineering, University of California San Francisco
2019 - 2022

Postdoctoral scholar, Andrej Sali lab

- **Protein structure modeling using chemical crosslinks**: Modeled macromolecular protein complexes by integrating homology models + mass-spectrometry derived chemical-crosslinks + cryo-EM data. Also developed graph sampling methods to learn domain boundaries in protein complexes from crosslink data. Applications include chromosomal maintenance (SMC5/6) and repair (DNA helicase) proteins
- **Computational mapping of nanobody epitopes**: Developed software to integrate chemical crosslink with escape mutation data for fast epitope determination of nanobodies on target proteins. Applications include epitope prediction of nanobodies on wild-type SARS-CoV-2 spike protein and its variants of concern
- **Whole cell models**: Developed Dynamic Bayesian Network (DBN) models to combine continuum scale (pharmacokinetic), particle scale (Brownian dynamics) and network scale (enzyme pathways) models of the pancreatic beta cell to build a proof-of-concept multimodal digitial twin of the beta cell. Served as software lead within the Pancreatic Beta-Cell consortium (collaborating across UCSF, USC, ShanghaiTech and HUJI)

Chemical Engineering, University of California Santa Barbara
2013 - 2018

PhD candidate, Shell lab

- **Thesis**: Next-Generation Coarse-Grained Models for Molecular Dynamics Simulations of Fluid Phase Equilibria and Protein Biophysics Using the Relative Entropy
- **Coarse-graining algorithms for bulk liquids**: Introduced the local density potential for structurally and thermodynamically accurate coarse-grained MD simulations of liquid-liquid phase separation, which are relatively rare in the chemical engineering literature
- **Coarse-graining algorithms for protein folding**: Developed protein backbone models for (i) template-free folding of 200+ residue coarse-grained protein domains using MD simulations, and (ii) studying self-assembly in amyloidogenic peptides
- **High Performance Computing**: System administrator for the Shell lab at UCSB (2016-2018). Set up 144 core Linux (Rocks 6.2) cluster and wrote utilities for automating (i) network-attached-storage management, and (ii) conflict-free compute resource sharing between lab members.

Volunteer

Peer-reviewer
2019 - Present

Structure, Review of Scientific Instruments, Rapid Reviews Covid-19, Life, Biomolecules, International Journal of Molecular Sciences

Co-founder, Graduate Simulation Seminar Series, UCSB
2014 - 2016

Conception, organization, public outreach and long-term funding support from ChE, Materials Science and Computer Science departments.

Research Interests

Protein design

Forcefield development

Amyloidogenic self assembly

Whole cell models

Bayesian networks

Variational inference

Selected Publications

Highly synergistic combinations of nanobodies that target SARS-CoV-2 and are resistant to escape
F.D. Mast, P.C. Fridy, N.E. Karen, J. Wang, E.Y. Jacobs, J.P. Olivier, T. Sanyal, et al, *eLife*, 2021

Bayesian metamodeling of complex biological systems across varying representations
B. Raveh, L. Sun, K.L. White, T. Sanyal, et al, *PNAS*, 2021

Integrative analysis reveals unique structural and functional features of the Smc5/6 complex
F.D. Mast, P.C. Fridy, N.E. Karen, J. Wang, E.Y. Jacobs, J.P. Olivier, T. Sanyal, et al, *PNAS*, 2021

A hybrid, bottom up, structurally-accurate, Go-like coarse-grained protein model
T. Sanyal, J. Mittal & M. Scott Shell, *JCP*, 2019

Transferability of local density-assisted implicit solvation models for homogeneous fluid mixtures
D. Rosenberger, T. Sanyal, M.S. Shell & N.F.A. van der Vegt, *JCTC*, 2019

Transferable coarse-grained models of liquid-liquid equilibrium using local density potentials optimized with the relative entropy
T. Sanyal & M. Scott Shell, *JPC-B*, 2018

Coarse-grained models using local-density potentials optimized with the relative entropy: Application to implicit solvation
T. Sanyal & M. Scott Shell, *JCP*, 2016

Recent conference presentations

7th Annual Computational Drug Development for Biologics Summit, Boston, MA, USA
(Talk): *Unpacking a workflow for automating protractor placement on peptides for enhanced half life*, Oct-2022

44th Indian Biophysical Society Meeting, Navi Mumbai, India
(Talk): *Integrative modeling of higher order complexes from binary binding modes*, Apr-2022

Biophysical Society Annual Meeting, San Francisco, CA, USA
(Talk): *Rigid body assignment in integrative determination of protein complex structures*, Feb-2022

PDB50: A special symposium celebrating the 50th anniversary of the Protein Data Bank, (virtiual)
(Poster): *Integrative modeling of the SMC5/6 complex*, May-2021

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

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

Awards

IUPAB best orgal presentation
44th Indian Biophysical Society Meeting

Technopreneurship Promotion Programme
Ministry of Science and Technology, Govt. of India

Seed money for prototype scale-up of bioreactors for algal biodiesel generation

Jagdis Bose National Science Talent Search (JBNSTS) fellowship