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**: Combined Homology models + chemical-crosslinks + cryo-EM data for protein complex structure modeling; graph sampling methods to extract domain information from crosslinks. Applications include SMC and DNA helicase protein families.
- **Computational mapping of nanobody epitopes**: Developed software to integrate chemical crosslinks with escape mutation data for protein-protein docking. Applications include epitope prediction of nanobodies on wild-type SARS-CoV-2 spike and variants.
- **Whole cell models**: Developed Bayesian Network models to combine continuum scale (pharmacokinetic), particle scale (Brownian dynamics) and network scale (enzyme pathways) models of the pancreatic beta-cell into build a proof-of-concept multimodal digitial twin 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**: As system administrator, 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.

Research Interests

Protein design

Forcefield development

Amyloidogenic self assembly

Whole cell models

Bayesian networks

Variational inference

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.

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

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

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