Tanmoy Sanyal

Scientist, Protein Design | Structural biology

About

San Francisco Bay Area, CA

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Protein Design

Rosetta AlphaFold RFDiffusion **ProteinMPNN**

Molecular modeling

openMM LAMMPS **GROMACS** IMP Modeller UCSF ChimeraX **PyMOL**

MI frameworks

PyTorch Tensorflow-probability PyMC3

Languages

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

Open Source

nbspike Integrative epitope prediction

IMP Crosslink guided domain discovery

PDB-Dev deposition Structure of SMC5/6

LAMMPS Local density potential

Education

University of California Santa Barbara

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

Kharagpur, WB, India

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

Research Experience

2023 - Present Amgen

Principal protein design scientist

Novo Nordisk Research Center Seattle

Protein design scientist

protraction.

Biologics design: (i) Design of mini-proteins and antibodies for multiple therapy areas using Rosetta and AlphaFold / RFDiffusion / ProteinMPNN pipelines (ii) SAR analysis based on protein language models. (iii) Optimizing non-canonical modifications to peptides for half-life

Scientific software development: Worked closely with AWS to re-tool AlphaFold and deploy a faster cloud-native in-house version for robust and scalable (~100k sequences) structure prediction; reguarly applied now in variant design within the company.

Department of Bioengineering, University of California San Francisco

Postdoctoral scholar, Andrej Sali lab

Protein structure modeling using chemical crosslinks: Homology models + chemicalcrosslinks + 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.

- Nanobody biophsyics: Developed integrative docking scores for nanobody docking on target receptors (SARS-CoV-2 and variant spike proteins) using chemical crosslinking and escape mutation data. Developed design principles for increasing nanobody thermostability.
- 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

PhD candidate. Shell lab

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 using variational inference techniques: Developed protein backbone models for (i) template-free folding of 200+ residue coarsegrained 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.

2013 - 2018

2008 - 2013

2022 - 2023

2019 - 2022

2013 - 2018

Research Interests

Volunteer

Protein language models

Peer-review

Integrative structure modeling

Non-canonical amino acids

Nanobodies

Forcefield development

Structure, Journal of Physical Chemistry, Proteins: Structure, Function and Bioinformatics, Review of Scientific Instruments, Rapid Reviews Covid-19, Life

Graduate Simulation Seminar Series, University of California Santa Barbara

2014 - 2016

2019 - Present

Co-founder

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 oral presentation

2022

44th Indian Biophysical Society Meeting

Technopreneurship Promotion Programme

2009

Ministry of Science and Technology, Govt. of India Seed money for prototype scale-up of bioreactors for algal biodiesel generation

2009

Jagdis Bose National Science Talent Search (JBNSTS) fellowship