Tanmoy Sanyal

Scientist, Computational Drug Design & Structural biology

About

Greater Seattle area, WA

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tanmoy7989

Structure prediction pipelines

AlphaFold
RFDesign
RFDiffusion
ProteinMPNN

Molecular modeling

Rosetta
openMM
LAMMPS
GROMACS
IMP
Modeller
UCSF ChimeraX
PyMOL

ML frameworks

PyTorch
Tensorflow-probability
PyMC3

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*
Protein design scientist

- **Biologics design**: Design of mini-proteins and antibodies for multiple therapy areas using Rosetta and AlphaFold / RFDdesign / RFDiffusion / ProteinMPNN pipelines, SAR analysis based on protein language models.
- **Method development**: MD forcefield design of non-canonical amino acid modifications to peptides, for mechanistic studies of half-life protraction.
- **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.
- **Leadership**: (i) Program lead for refining protein interface prediction ML models in collaboration with the Institute for Protein Design at UW, Seattle. (ii) Led and evaulated a proof of concept for onboarding virtual reality based structural rendering software among collaborative teams of computational design scientists and synthetic chemists.

Department of Bioengineering, University of California San Francisco *2019 - 2022*
Postdoctoral scholar, Andrej Sali lab

- **Protein structure modeling using chemical crosslinks**: 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.
- **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 *2013 - 2018*
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 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

Non-canonical amino acids

Forcefield development

Amyloidogenic self assembly

Whole cell models

Bayesian networks

Variational inference

Volunteer

Peer-review *2019 - Present*

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*

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

Jagdis Bose National Science Talent Search (JBNSTS) fellowship *2009*