Ilan E. Chemmama

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Google Scholar Profile

QUALIFICATION SUMMARY

Structural biologist, programmer, and software engineer experienced in using Bayesian inference for biology

- Inferring structure macromolecular assemblies of various sizes and scales by integrative modeling
  - Contributed to the determination of the structures of eight macromolecular assemblies
  - Maximized accuracy and precision by simultaneously utilizing all available information, including experimental data, physical principles, statistical analyses, and other prior models
  - Used sample-based Bayesian inference to generate models that satisfy the input information
  - Used high-performance scientific computing to efficiently sample those models
  - Estimated uncertainty originating from information that is sparse, noisy, ambiguous, or derived from heterogeneous samples
  - Developed and applied a pipeline to assess sampling convergence for stochastic sampling
  - Developed, implemented, and contributed code for data analyses in C++ and Python to the open-source software *Integrative modeling platform* (IMP) package
- Strong communication and collaboration skills
  - Collaborated with large and small multidisciplinary teams of scientists to produce peer-reviewed publications, conference presentations, and successful competitive grant proposals
  - Mentored high school, undergraduate, and graduate students

RELEVANT RESEARCH EXPERIENCES

Computational Structural Biology

University of California - San Francisco, San Francisco, CA USA 2013 to Present

Inferring structures, free energy differences, and kinetic rates of biological macromolecular assemblies by integrative modeling

Principal Investigator: Prof. Andrej Sali

- *Computing integrative atomic structures based on medium-resolution EM density maps:* Biomolecular structures are routinely computed based on their electron microscopy (EM) density maps. The accuracy and precision of such modeling depends critically on a scoring function that quantifies a match between a model and the map. We introduce a Bayesian posterior model density for a model given its map, explicitly taking into account the resolution and other uncertainties in the map.
- *Structural dynamics of the human Cop9 signalosome:* The COP9 signalosome (CSN) is an evolutionarily conserved eight-subunit protein complex that controls protein ubiquitination by deneddylating Cullin-RING E3 ligases. The activation and function of CSN hinges on its structural dynamics, which has been challenging to decipher by conventional tools. We determined the structural dynamics of the human Cop9 signalosome complex by integrative modeling, demonstrating how the synergy between multi-chemistry cross-linking mass spectrometry and integrative modeling can map the structural dynamics of macromolecular assemblies.
- *Inferring free-energy differences and kinetic rates of biomolecules:* Mapping the functional cycle of a biomolecular machine requires determining the structures of key states, their stabilities, and the kinetics of their interconversions under native conditions. We describe a method that outputs these free-energy differences and kinetic rates based on time-dependent negative-stain electron microscopy particle images for a given set of structural states and transitions between them. We illustrate our method by applying it to the yeast Hsp90 chaperone engaged in its ATPase cycle in the presence of two ATP analogs, the non-hydrolysable AMP·PNP or the slowly hydrolysable ATPγS.

- *Validation of stochastic sampling in integrative modeling:* Modeling of macromolecular structures involves structural sampling guided by a scoring function, resulting in an ensemble of good-scoring models. By necessity, the sampling is often stochastic, and must be exhaustive at a precision sufficient for accurate modeling and assessment of model uncertainty. We present an objective and automated method for validating and assessing stochastic sampling in integrative modeling.
- *3D structures determination of biological assemblies of various sizes and scales by integrative modeling:* Leveraging multiple sources of information (*e.g.* cross-linking mass spectrometry, 2D EM images, 3D EM maps, among others), I contributed to the structure determination of · the yeast exocyst complex, · the human ECM29-Proteasome assembly under oxidative stress, · the yeast nuclear pore complex (NPC) cytoplasmic mRNA export platform, · the major membrane ring component of the yeast NPC, · the entire yeast NPC, and · the reconstruction of 3D structures of MET antibodies.

THEORETICAL BIOPHYSICS 2008-2013
Florida International University, Miami, FL USA

Physics of small peptide folding and the formation of secondary structures

Principal Investigators: Profs. Bernard S. Gerstman and Prem P. Chapagain

- *Structural propensities and entropy effects in peptide helix-coil transitions:* The helix-coil transition in peptides is a critical structural transition leading to functioning proteins. Peptide chains have a large number of possible configurations that must be accounted for in statistical mechanical investigations. Using hydrogen bond and local helix propensity interaction terms, we develop a method for obtaining and incorporating the degeneracy factor that allows the exact calculation of the partition function for a peptide as a function of chain length.
- *Pairwise amino acid secondary structural propensities:* We investigate the propensities for amino acids to form a specific secondary structure when they are paired with other amino acids. Our investigations use molecular dynamics (MD) computer simulations, and we compare the results to those from the Protein Data Bank (PDB). Proper comparison requires weighting of the MD results in a manner consistent with the relative frequency of appearance in the PDB of each possible pair of amino acids.

EDUCATION

PH.D. IN BIOPHYSICS March 2020
University of California - San Francisco, San Francisco, CA USA

Thesis: "Inferring structures, free-energy differences, and kinetic rates of biological macromolecular systems by integrative modeling." *Advisor*: Andrej Sali
National Science Foundation Graduate Research Fellow

BACHELOR OF SCIENCE IN PHYSICS May 2011
Florida International University, Miami, FL USA

Honors Thesis: "Theoretical Quantification of Self-Organization of Secondary Interactions in Protein Folding." *Advisors*: Bernard S. Gerstman and Prem P. Chapagain
Graduated with minors in Chemistry and Mathematics
Graduated *Magna Cum Laude*, Honors Course of Study in Physics, and through *The Honors College*.

SELECTED PUBLICATIONS (OUT OF 13)

Structural dynamics of the human COP9 signalosome revealed by cross-linking mass spectrometry and integrative modeling
Proceedings of the National Academy of Sciences Feb 2020, 117 (8) 4088-4098
Craig Gutierrez*, **Ilan E Chemmama***, Haibin Mao, Clinton Yu, Ignacia Echeverria, Sarah A Block, Scott D Rychnovsky, Ning Zheng, Andrej Sali, Lan Huang

Assessing exhaustiveness of stochastic sampling for Integrative Modeling of macromolecular structures
Biophys. J. 113, 2344-2353 (2018)
Shruthi Viswanath*, **Ilan E. Chemmama***, Peter Cimermancic, and Andrej Sali

Pairwise amino acid secondary structural propensities
Phys. Rev. E 91, 042709 (2015)
Ilan E. Chemmama, Prem P. Chapagain, and Bernard S. Gerstman

Structural propensities and entropy effects in peptide Helix-Coil transitions
Phys. Rev. E 86, 031915 (2012)
Ilan E. Chemmama, Adam Colt Pelea, Yuba R. Bhandari, Prem P. Chapagain, and Bernard S. Gerstman

SELECTED LIST OF AWARDS

National Science Foundation Graduate Research Fellow
University of California - San Francisco, 2015

The Phi Beta Kappa Society
Epsilon Chapter of Florida, 2011

SELECTED PRESENTATION AND CONFERENCES ATTENDED

Towards modeling multiple states of biomolecules satisfying spatial restraints from single-particle EM images
Ilan E. Chemmama 6-10 May 2017
World Molecular Engineering Conference, Cabo San Lucas, Mexico

Towards modeling multiple states of biomolecules by satisfaction of spatial restraints from single-particle electron microscopy images
Ilan E. Chemmama, Charles H. Greenberg, and Andrej Sali 11-15 February 2017
61st Annual Meeting of the Biophysical Society, New Orleans, LA USA

Theoretical and computational quantification of self-organization of secondary interactions in protein folding
Ilan E. Chemmama, Prem P. Chapagain, Bernard S. Gerstman, Jose L. Parra 31 March to 2 April 2011
National Conference for Undergraduate Research, Ithaca, NY USA

OUTREACH AND TEACHING EXPERIENCES

Volunteer for JUMA Ventures
San Francisco, CA USA January 2016 to Present
Juma strives to break the cycle of poverty by paving the way to work, education, and financial capability for youth across America. I am a STEM tutor where I mentor students in science and mathematics (Algebra, Statistics, and Calculus, Chemistry) as well as SAT/ACT prep.

Volunteer for the Overtown Youth Center
Miami, FL USA June 2010 to August 2013
I was a volunteering tutor for a partnership established by Dr. Jayne Klein between the Honors College at Florida International University - Biscayne Bay Campus and the Overtown Youth Center. Overtown is Miami's most economically disadvantaged neighborhood. The partnership provides youth attending the center opportunities to build competency in English, mathematics, and critical thinking skills, with the aim of improving their access to higher education. I often used science as an anchor for students to stimulate their interest in science and mathematics.

Research Mentorship
UCSF, CA USA 2015 to present
I mentored two first-year graduate students rotating in the Sali lab and two high-school students doing summer internships

Teacher Assistant
UCSF, CA USA 2014-2017
I was a teacher assistant for *Macromoleculess, Structures, and Interactions A* and the *NSF Writing Class*

Instructor for the Department of Physics
FIU, FL USA January 2010 to July 2013
I taught various sections of classes for first and second-year level astronomy and physics courses and laboratories.