

Feb 18th, 10:15 AM - 11:15 AM

Oral Concurrent Session II: Interdisciplinary Research in Computer Science, Biology, and Physics

Jing He
Old Dominion University

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10:15-11:15 AM (ROOM 1310)

Interdisciplinary Research in Computer Science, Biology, and Physics

Chair: Dr. Jing He, Computer Science

Comparing an Atomic Model or Structure to a Corresponding Cryo-EM Image at the Central Axis of a Helix

Stephanie Zeil & Devin Haslam (Mentor: Drs. Jing He, Willy Wriggers, and Julio Kovacs)

Three-dimensional density maps of biological specimens from cryo-electron microscopy (cryo-EM) can be interpreted in the form of atomic models that are modeled into the density, or they can be compared to known atomic structures. When the central axis of a helix is detectable in a cryo-EM density map, it is possible to quantify the agreement between this central axis and a central axis calculated from the atomic model or structure. We propose a novel arc-length association method to compare the two axes reliably. This method was applied to 79 helices in simulated density maps and six case studies using cryo-EM maps at 6.4-7.7Å resolution. The arc-length association method is then compared to three existing measures that evaluate the separation of two helical axes: a two-way distance between point sets, the length difference between two axes, and the individual amino acid detection accuracy. The results show that our proposed method sensitively distinguishes lateral and longitudinal discrepancies between the two axes, which makes the method particularly suitable for the systematic investigation of cryo-EM map-model pairs.

Modelling Beta-sheets using Iterative Bézier Surface Fitting on Cryo-EM Density Maps

Michael Poteat (Mentor: Dr. Jing He)

Cryo-electron microscopy is a powerful technique to produce 3-dimensional images for large molecular complexes. When the resolution of 3-dimensional images is not sufficient to derive atomic structure directly from the image, it is still challenging to interpret the image. In order to model β -strands from medium-resolution images, we propose the use of Bézier surface iteratively to fit a β -sheet image. The proposed method shows improved accuracy in fitting when it was tested using eight cases.

Challenges in Matching Secondary Structures in Cryo-EM – An Exploration

Devin Haslam (Mentors: Drs. Mohammed Zubair, Desh Ranjan, and Jing He)

Cryo-electron microscopy is a fast emerging biophysical technique for structural determination of large protein complexes. While more atomic structures are being determined using this technique, it is still challenging to derive atomic structures from density maps produced at medium resolution when no suitable templates are available. A critical step in structure determination is how a protein chain threads through the 3-dimensional density map. A dynamic programming method was previously developed to generate K best matches of secondary structures between the density map and its protein sequence using shortest paths in a related weighted graph. We discuss

challenges associated with the creation of the weighted graph and explore heuristic methods to solve the problem of matching secondary structures.

Development of a Software Tool for Protein Secondary Structure Detection from Electron Density Maps from Cryo-Electron Microscopy

Christopher Spillers (Mentor: Drs. Jing He, and Willy Wriggers)

The accuracy of the secondary structure identification from volumetric protein density maps is critical for de-novo backbone structure derivation in electron cryo-microscopy (cryoEM). It is still challenging to detect the SSE automatically and accurately from the density maps at medium resolutions. Various computational methods exist in secondary structure detection with strengths and weaknesses. The goal of this work is to combine two computational methods *SSETracer* and *Voltrac* in one software tool for enhanced detection. A framework of a user-interactive software tool has been established incorporating the strength from the above two methods.

Improving the Efficiency of Compton Scattering Calculations

John Rattz (Mentor: Drs. Balsa Terzic, Mohammed Zubair, and Desh Ranjan)

Compton or Thomson scattering can be used in constructing sources of high energy photons. In recent years there has been a revival of activity in the subject driven by the desire to produce several keV X-ray sources from relatively compact relativistic electron accelerators. Such sources are attractive due to the narrow bandwidth generated in the output radiation. We have developed a calculation method yielding the energy spectral distribution of the radiation produced by the scattering event, and extended it so that the radiation from a group of relativistic electrons may be obtained. The heart of the project was a program that performed an adaptive 2D integration. The goal was to improve the program's performance by translating it from Python to C++. There were several differences between how the two implementations performed the same task, with these differences being relevant to the program's performance.