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Structure Determination from Single-Particle X-ray Imaging

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X-ray free electron lasers, such as Linac Coherent Light Source at SLAC, can be used to generate diffraction patterns of non-crystalline biological objects, like viruses. Then the main goal is to extract the high-resolution 3D structure of such particles by assembling 2D diffraction data with random orientations. However, structure determination still remains as a major challenge, and powerful algorithms are in high demand. We present a new approach for reconstructing the 3D anatomy of symmetric objects such as viruses, using simulated random diffraction snapshots generated by X-ray free electron lasers. We show that a manifold embedding technique is able to determine the orientations of diffraction patterns of a small virus with sufficient accuracy for atomic-level reconstruction of its structure. We also discuss challenges and possibilities in structural recovery of macromolecules from the experimental X-ray data.

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