Exhaustive Parameter Space Searches in Cryo-Electron Microscopy using GPU

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Open and Closed state of HIV spike – 24 Å tomography

A typical tomography subvolume

\[ SNR = \frac{\sigma_s}{\sigma_n} \approx 0.25 \]
Nuclear Norm allows one-versus-many comparison

\[ \|A\|_* = \sum_{i=1}^{n} \lambda_i(A) \]

\( \lambda_i(A) \) - singular values of A

- Incremental SVD update/downdate

\[ \begin{bmatrix} Ab \end{bmatrix} \cdot \begin{bmatrix} Ab \end{bmatrix}^T = A \cdot A^T + b \cdot b^T \]

- is \( O(n^2) \) as compared to \( O(n^3) \) of SVD
- can be efficiently implemented in GPU
Near-Atomic Single Particle Reconstruction
E-coli beta-galactosidase - 3.2 Å
Thank you!