Ethan Suwandi
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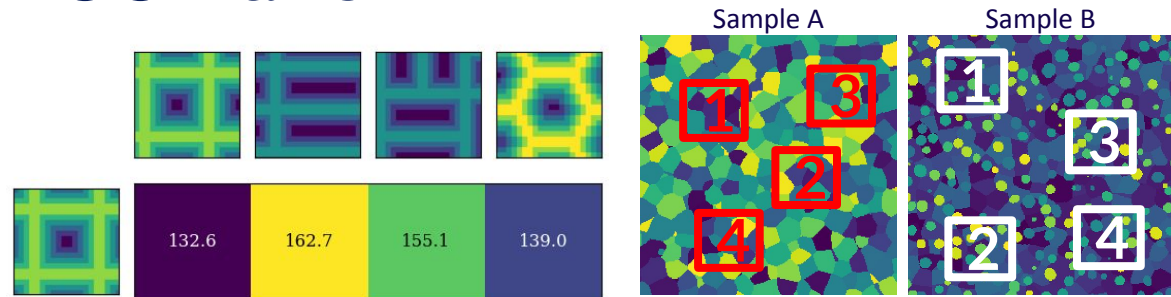
Microstructure Comparison via the Wasserstein Metric

Single Comparison Metric

Local Morphology

Reduces many physical descriptors

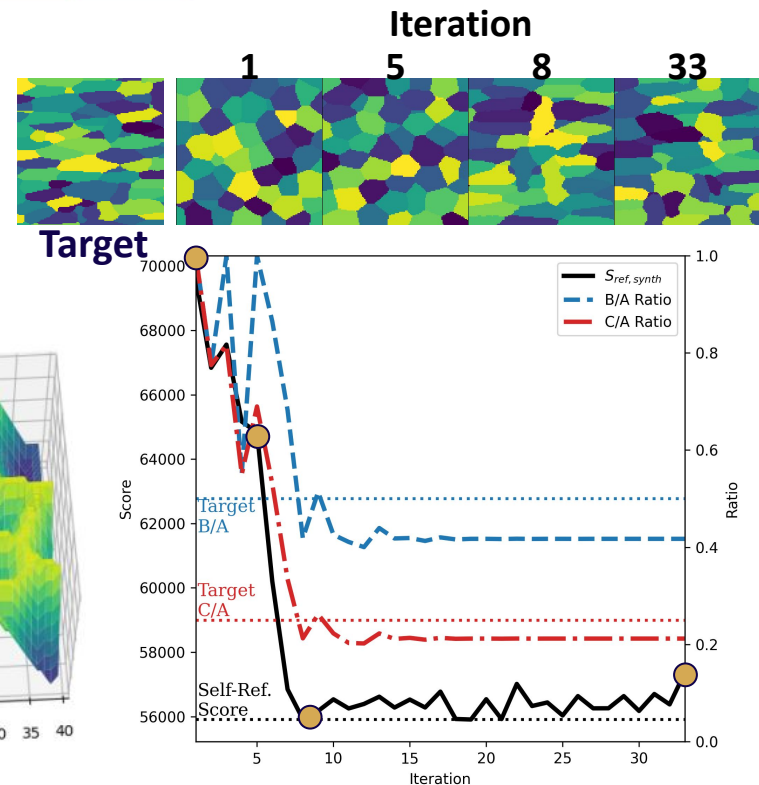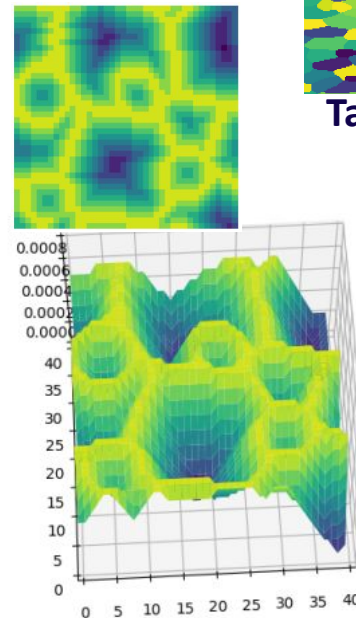HPC Usage: Parallelization of window comparisons (NxN).

BIV RNA-Peptide Mutant Data Analysis

Large Scale Conformational and MD Simulations

High Dimensional Data

Analysis of multiple simultaneous simulations.

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Computational Challenges

- Planning for parallel use at the beginning.
- Proper project structure and expandability.
- Visualization of Large Scale/High Dim. Data.
- Strengths, Weaknesses, and proper HPC use.

75-0006 flex
Total HB: 9139
Protein Poses: 842

3: 0.49%   G — C   30: 0.12%
4: 0.85%   G — C   29: 0.19%
5: 2.64%   C — G   28: 0.49%
6: 11.57% U — A   27: 0.80%
7: 9.15%   C — G   26: 2.56%
8: 13.75% G — C   25: 3.78%
9: 8.00%   U
10: 1.06% G   C   24: 12.45%
11: 1.83% U   23: 7.39%
12: 1.29% A
13: 1.24% G   C   22: 4.63%
14: 0.86% C   G   21: 5.89%
15: 0.67% U   A   20: 4.42%
                       19: 1.96%
16: 0.20% C   18: 0.97%
17: 0.77% A   U