Summary 1st day

Model building

Objective

To construct accurate 3D atomic models of biomolecules (typically proteins) based on experimental or predicted data, enabling insights into their function, interactions, and mechanisms.

Map Preprocessing: enhance map sharpness

One effective approach is local filtering (LocalDeblur), which adaptively enhance features based on local resolution.

Initial Model

- Alphafold
  - AI-based
  - Highly accurate, especially for single-chain proteins (5000)
  - No experimental structure is used
- ModelAngelo
  - Integrates deep learning and structural constraints
  - Works better at resolution less than 3.5 Å
- Modeller (Sequence Homology Modeling)
  - Builds models based on known structures of similar sequences
  - Relies on evolutionary conservation
  - Effective when homologous templates are available