

Integrated Modelling of PROTEIN Complexes VIA Single Shot Registration using DREAM (IMPROVISeD)



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1. Integrative Modelling Platform (IMP)

- 1. The IMP provides a computational approach designed to model the structure of macromolecular assemblies.
- 2. It models large macromolecular complexes by integrating data from experiments, statistical analyses, physical principles, and prior models.

2. Drawbacks of IMP

- 1. Computationally expensive.
- 2. Uses Markov Chain Monte Carlo (MCMC) sampling.

3. Proposed Method

- 1. We propose to replace the MCMC sampling with a bottom-up approach.
- 2. We will use DREAM algorithm to replace the MCMC sampling.

4. Distance Restraints and Energy Assisted Modelling (DREAM)

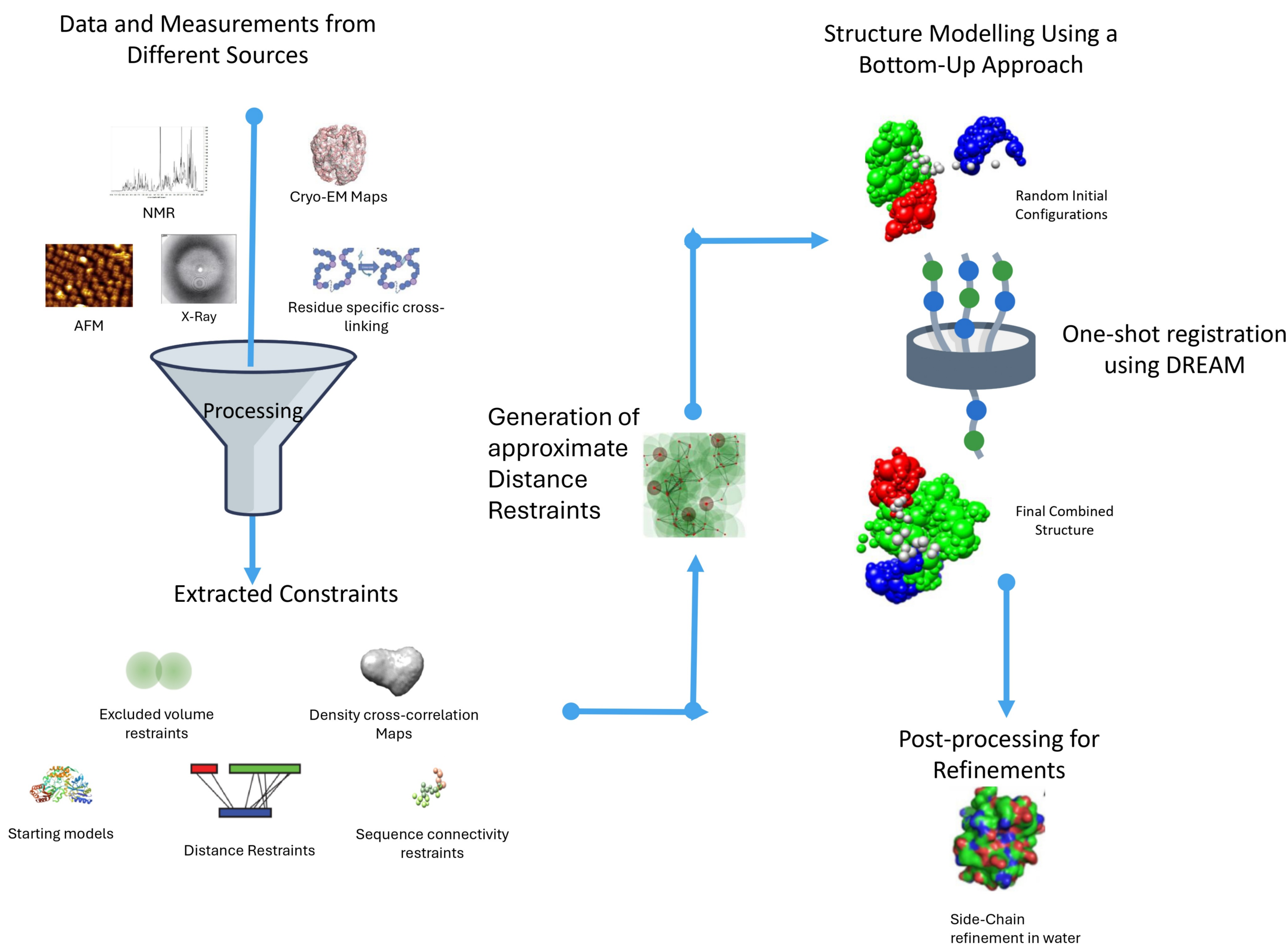
This algorithm takes distance restraints data and models the structure of proteins which includes 3 steps:

- 1. Constructing the substructures.
- 2. One shot registration of all the substructures.
- 3. Gap filling using hybrid approached.

Sub Topic 2

Enter content on subtopic

Graphical Overview



Conclusions and Future Work

Final conclusions

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