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

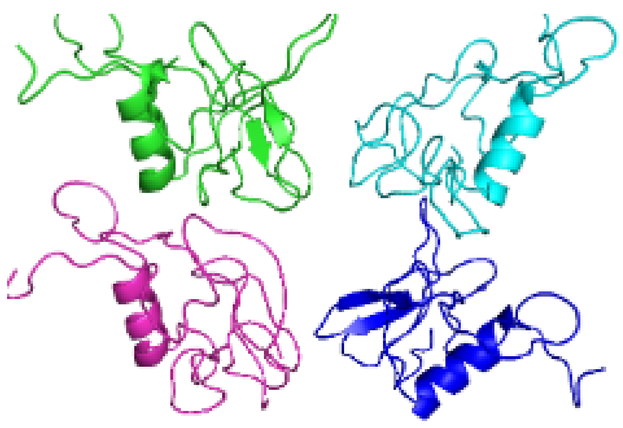
1. We propose to replace the MCMC sampling with a bottom-up approach.
2. We will use DREAM algorithm to replace the MCMC sampling.

4. Distance Restraints and Energy Assisted Modelling (DREAM)

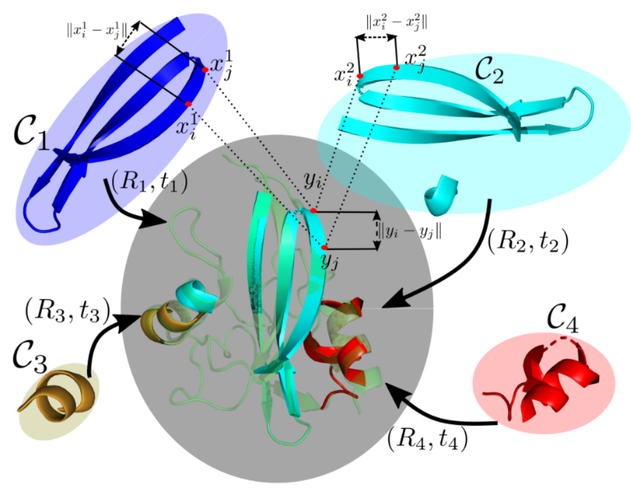
This algorithm takes distance restraints data and models the structure of proteins which includes 3 steps:

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

4.1 Substrucutre Construction

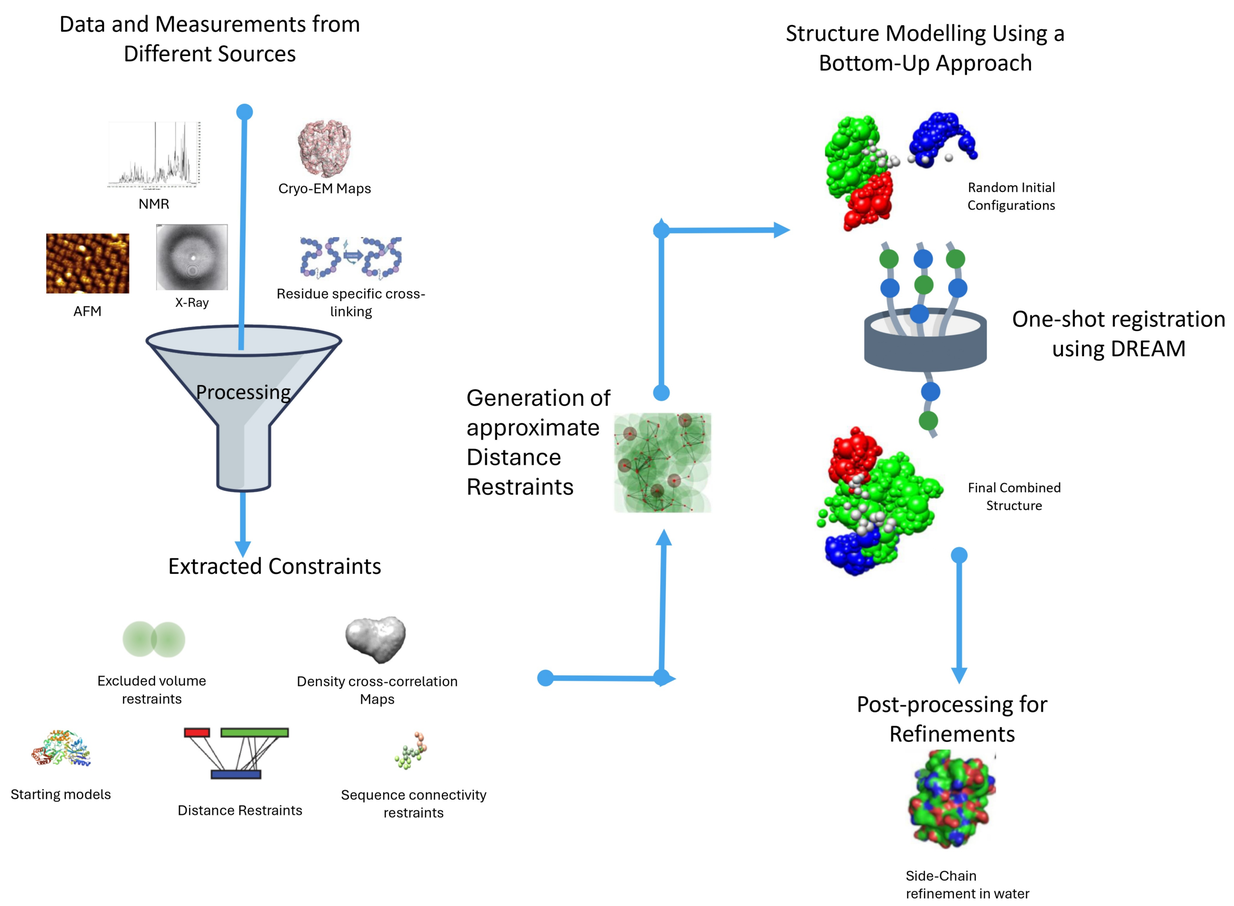


4.2 One-Shot Registration



4.3 Gap Filling

5. Graphical Overview of proposed method



6. Human Practices

3R's

1. Replacement
2. Reduction
3. Refinement

Our Stakeholders

1. Professors
2. Research Students
3. Protein Modelling Companies

7. Our Mentors

1. Professor Debnath Pal (CDS IISc)
2. Dr. Shruthi (NCBS)

8. Summary

1. Extract the distance restraints data from various experimental data.
2. Use principle of DREAM algorithm to model the structure of complex.
3. Generate the PDB file.

9. Links and Resources

SCAN ME