MOLECULAR IMAGE REGISTRATION USING MUTUAL INFORMATION AND DIFFERENTIAL EVOLUTION OPTIMIZATION

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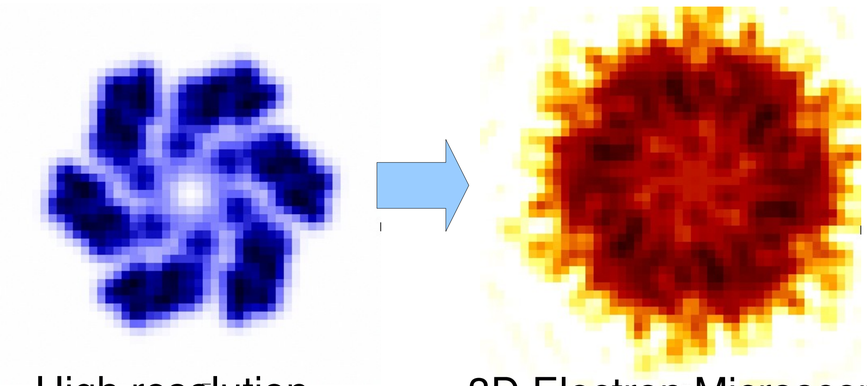
SUMMARY

- we developed algorithms for combining volumes of domains and macromolecular complexes to highlight how these pieces interact to perform their biological function
- the problem is stated in a form of rigid image registration
- we focus on image metrics and optimization techniques
- mutual information combined with two step optimization gives the best results

MOTIVATION

Goal: Efficiently and robustly localize known domains in three dimensional molecular complex

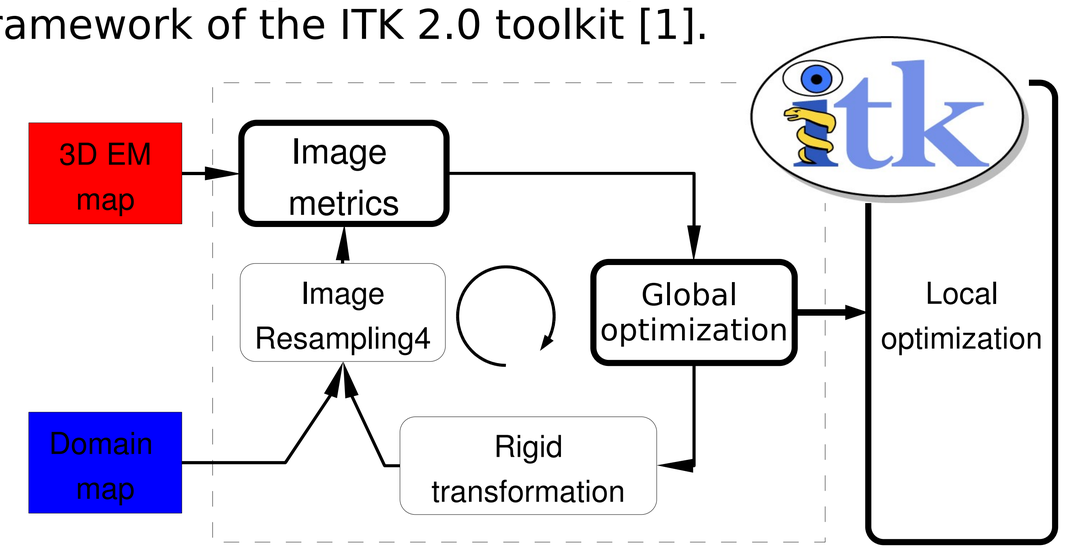


High resolution domain

3D Electron Microscopy reconstruction

METHODS

We aligned two images with the rigid registration algorithm. The quality of fit was evaluated using two voxel intensity based metrics: mutual information (MI) [3] or cross-correlation (CCC). The best parameters of transformation were found by two-step optimization involving evolutionary strategy followed by gradient search. The algorithms were implemented in the framework of the ITK 2.0 toolkit [1].



DIFFERENTIAL EVOLUTION

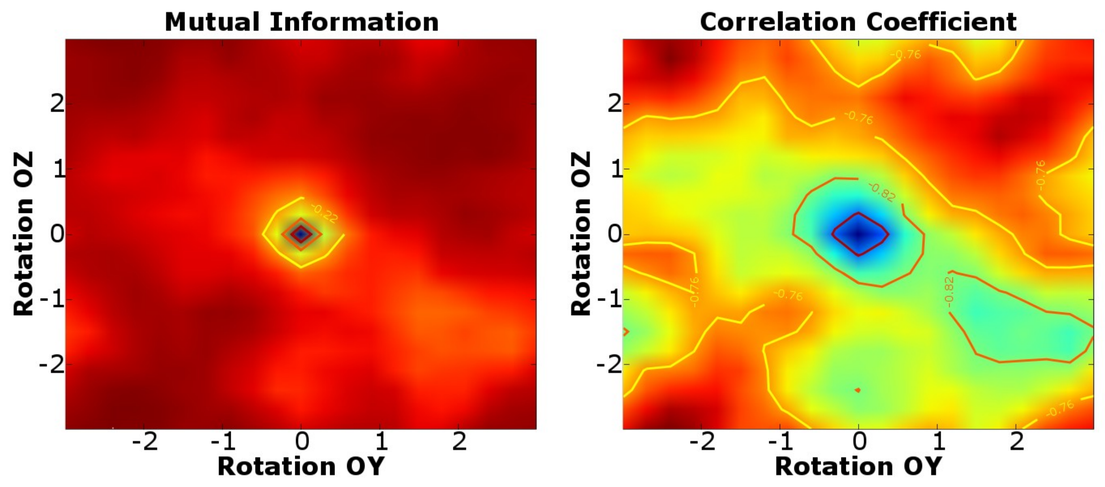
(1) Generate initial population of *NP* parameter vectors.
(2) Generate new vector:

$$\underline{v}_{i,G+1} = \underline{x}_{r_1,G} + F \cdot (\underline{x}_{r_2,G} - \underline{x}_{r_3,G})$$

(3) Perform crossing-over with probability CR.
(4) Evaluate objective function and compare it with random population member.
(5) Retain a vector with a lower value in the next generation [2].

RESULTS

The comparison of metrics value as a function of transformation parameters shows that MI is a more robust measure yielding, less local minima than the commonly used CCC.



We generated 20 random initial transformations (angles: $\pm\pi$ rad, translations: ±20 px) and for each of them we ran the registration procedure.

Correct Angle Domain	Correct Angle Molecule	Correct
Simulated		
PBD-1a8d02	PBD-1a8d	65%
Experimental		
PBD-1oelB1	MSD-1081	95%
PBD-1oelB2	MSD-1081	76%
PBD-1oelB3	MSD-1081	95%
PBD-1d2n	MSD-1059	86%

PROSPECTIVE RESEARCH

- incorporate the algorithm into molecular database searching to find the complete set of domains building the studied complex
- use additional preprocessing such as Laplace filtering to further improve accuracy and robustness of the algorithm
- extend the approach to more general classes of transformations (affine, non-rigid)

REFERENCES

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2. R. Storn, K. Price, *IEEE Conference on Evolutionary Computation*, 2006
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