Clustering for multi-crystal data collection

A tool for Synchrotron Serial Crystallography data processing

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Acknowledgements

- ESRF
  - Alexander Popov
  - Olof Svenson
  - Uli Zander
  - Igor Melnikov

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Hierarchical cluster analysis and protein crystallography

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HCA: introduction

A method to cluster large ensambles of data

- Distance matrix
  - Define distance between all pairs of datasets
  - Use unit cell variation
  - Correlation coefficient between datasets

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  - Correlation coefficient between datasets
- Linkage method
  - Complete linkage
  - Distance between clusters A and B: $max(d_{a,b}); a \in A, b \in B$
  - Gives upper limit of cluster quality

Definitions of distance

- According to unit cell variation
  - $d(a,b) = max(\frac{|A_a - A_b|}{min(A_a, A_b)}, \frac{|B_a - B_b|}{min(B_a, B_b)}, \frac{|C_a - C_b|}{min(C_a, C_b)})$
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  - A,B,C unit cell parameters of each dataset
- According to correlation
  - $d(a,b) = \sqrt{1 - cc_{a,b}^2}$
  - $cc_{a,b}$ correlation coefficient between datasets

Implementation of ccCluster

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  - Used cctbx.miller module
  - Can run on various file formats
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Correlation coefficients
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17   50   0.966456682722
17   21   0.558234058272
17   86   0.978797299202
17   62   0.959380884366
17   32   0.976804797012
17   40   0.983532727402
17   51   0.97603906066
17   85   0.923668052721
17   19   0.985738729727
17   65   0.982510403238
17   68   0.97893905106
17   23   0.960741701806
17   74   0.937200562712
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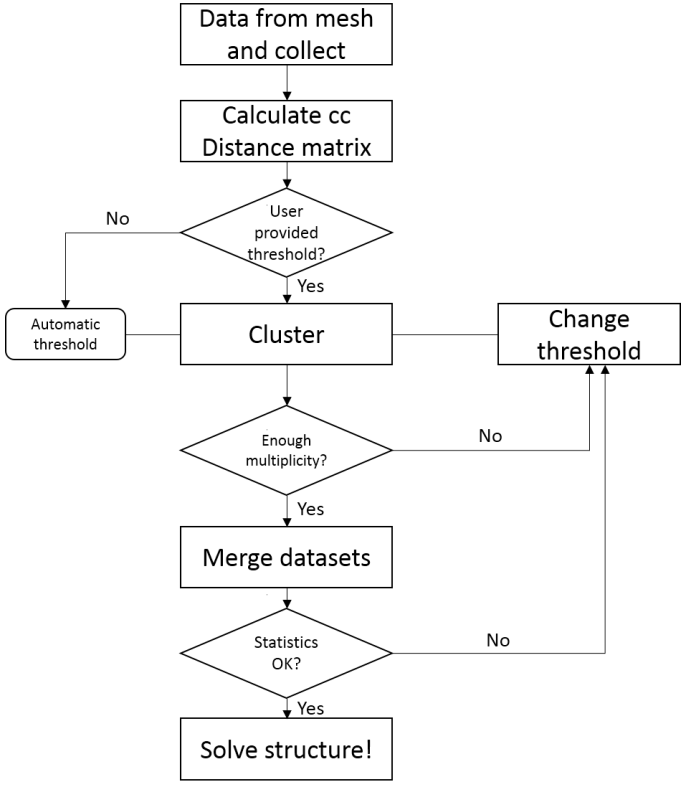

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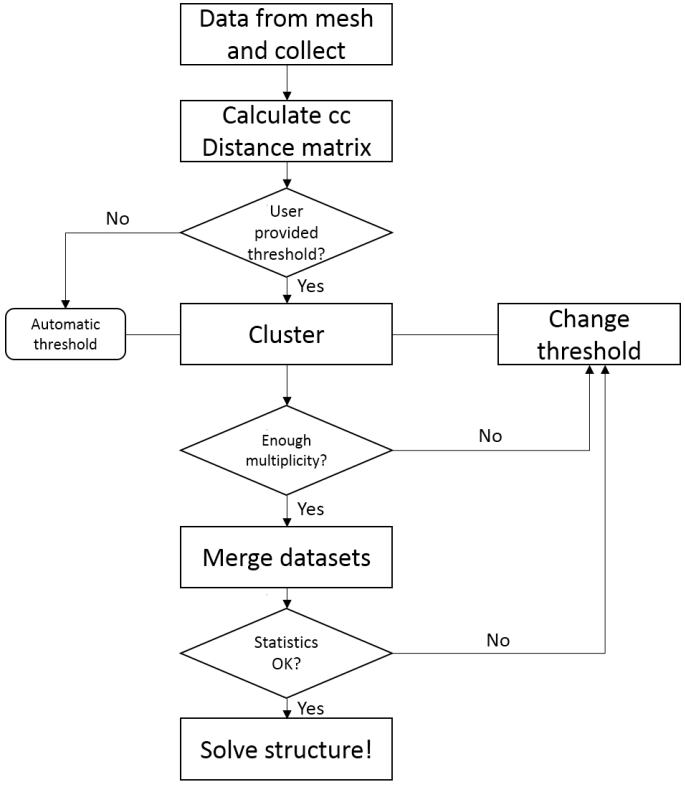

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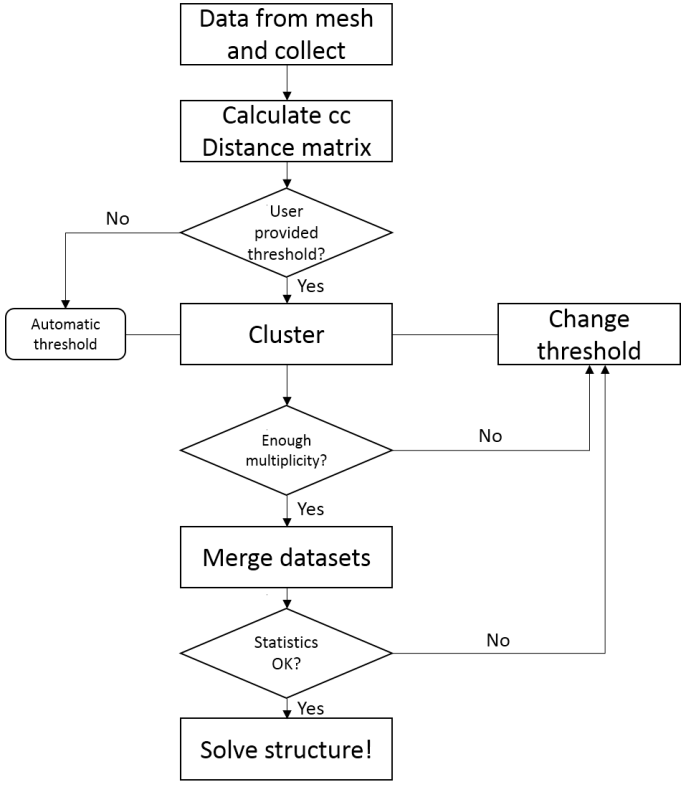

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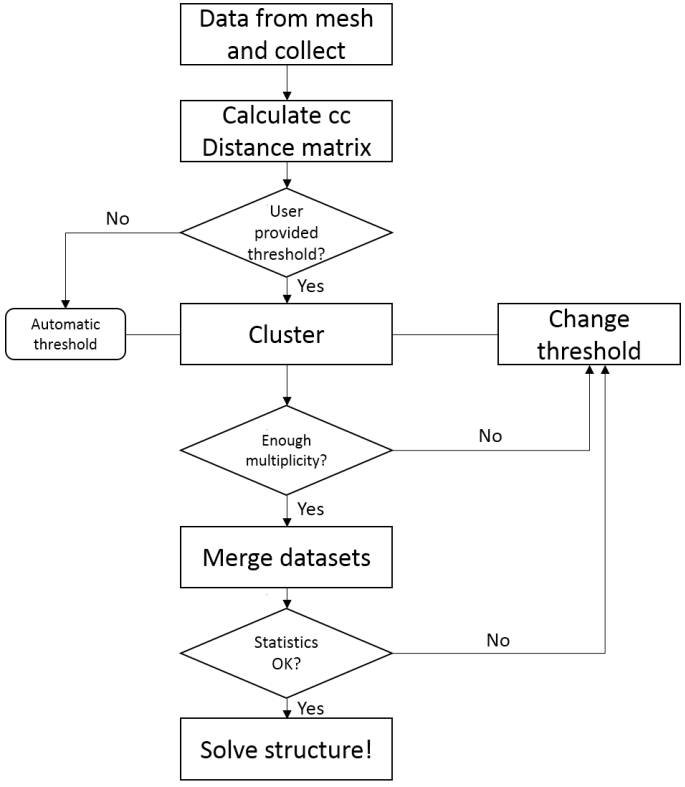
- Summary
  - Synthesis of the results
  - Suggests which cluster to chose, according to target



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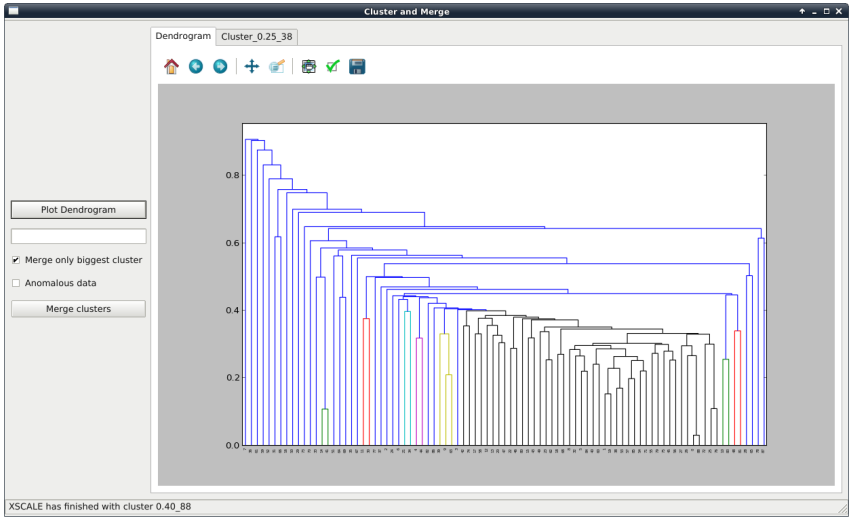

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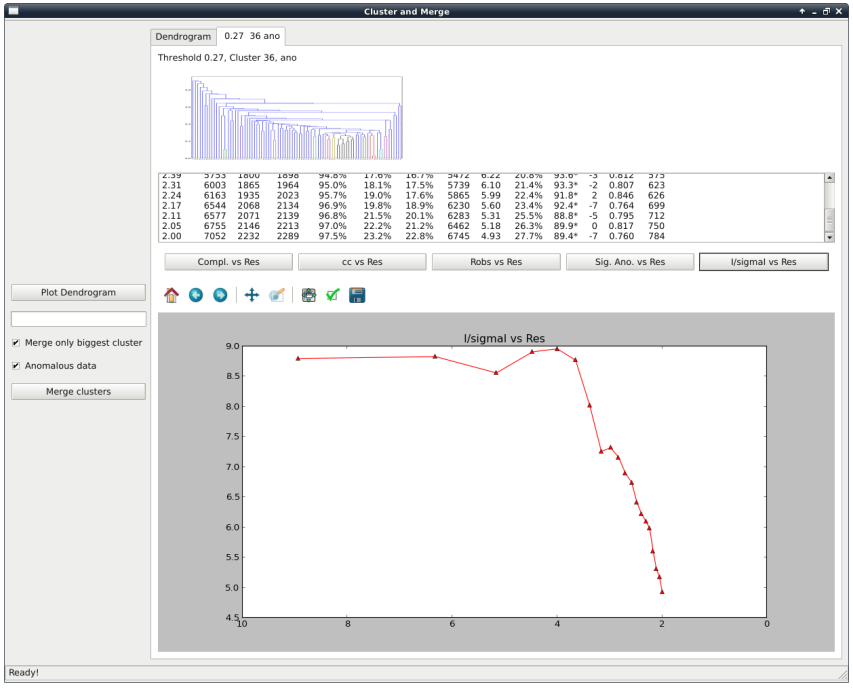

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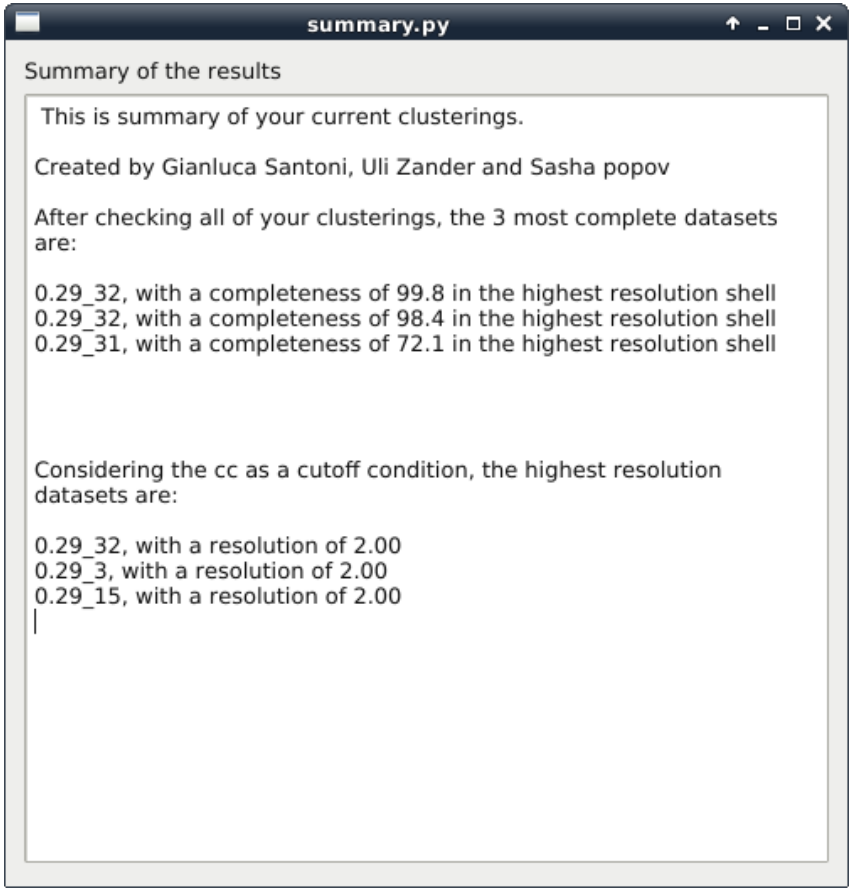

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Conclusion

What I talked about

- Promising first tests of clustering (as Uli showed)
- We can use cc and unit cell to compare datasets
- Clustering with cc has been tested widely for mesh and collect
- GUI of ccCluster is ready to use (please, ask if interested)

What I did not talk about

- Comparison between the two definitions of distances
  - Few common reflections or error in unit cell determination
  - Lowest angle wedges possible to be determined
- Other applications
  - SAD experiments
  - Weak diffracting / radiation sensitive crystals

Thank you

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