

Map manipulation

Exercises in map manipulation.

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Sienna/Map manipulation

Map manipulation

Exercises:

(Attempt any or all of these in any order. Don't expect to finish them during the meeting)

- Identify connected regions in a mask
- Skeletonise an electron density map
- Calculate electron density from atomic coordinates
 - Each task can be more or less difficult depending on whether you account for lattice repeat, space-group symmetry, and cell geometry.

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Sienna/Map manipulation

Map manipulation

Identify connected regions in a mask

- The file mask.txt contains a 12x10x8 mask, in obvious human readable format. Read this into an array, and using an algorithm of your choice, identify how many discrete connected masked regions there are. Mark each connected region in the mask with a unique identifier. Print a list of them, along with their sizes.
- For a more advanced solution, include the fact that the map is cyclic and wraps round at its edges.

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Sienna/Map manipulation

Map manipulation

Skeletonise an electron density map

- The file map.txt contains a 12x10x8 map, in obvious human readable format. Read this into an array, and calculate a modified Greer skeleton, using the algorithm described.
- For a more advanced solution, include the fact that the map is cyclic and wraps round at its edges.
If writing this using Clipper, you should also be able to incorporate crystallographic symmetry. (If you store the skeleton in an Xmap, then it will also have magic symmetry. This is how 'coot' displays infinite skeletons.)
- Are there any changes you would make to the program to support skewed grids?

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Map manipulation

Calculate electron density from atomic coordinates

- Using a blank 12x10x8 map representing a 18x15x9Å cell, read the coordinates from the file atoms.txt. Calculate the electron density for the unit cell, assuming that each atom is a Gaussian whose height is its atomic number and whose half width is 0.75Å.
- For a more advanced solution, include the fact that the map is cyclic and wraps round at its edges.
- How must the calculation be modified to handle skewed cells? What types of coordinates are involved?
- If you are using Clipper, the file clipper/contrib/edcalc.cpp contains a symmetry general solution: `Edcalc_iso<T>::operator()`. Why do you think a multiplicity correction is required at the end of the calculation?

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Skeletonisation:

- Aim is to trace the ridges connecting peaks of density in the map.
- Simplest approach is a modified 'Greer' algorithm.
 - This version descended from one implemented in 'dm' in the late '90s.
 - Also similar to one used in TEXTAL.
- A more general version (symmetry and crystal geometry) is implemented in Clipper.

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Sienna/Map manipulation

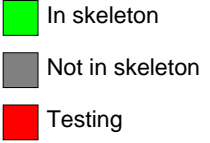
Map manipulation

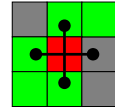
Skeletonisation:

- Make a map of flags, using the same grid as the density map. Mark every point as 'skeleton'.
- Consider each grid point in the map in turn, in order of increasing density.
 - For each point, consider whether removing that point from the skeleton will 'disconnect' any of its (6 orthogonally adjacent) neighbors.
 - If so, leave it in the skeleton.
 - If not, remove it from the skeleton.

Map manipulation

Skeletonisation:

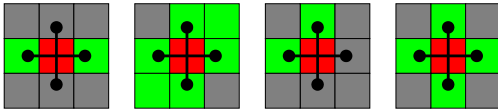
- e.g. in 2 dimensions...
 - 
- So in this example, removing the center point will disconnect the top neighbor from the left and bottom neighbors.
 - So we keep it.



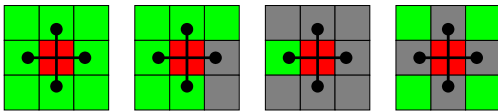
Map manipulation

Skeletonisation:

- Keep:



- Lose:



Map manipulation

Skeletonisation:

25	3	8	24	17	18
21	7	29	14	11	28
10	30	23	13	6	20
4	15	16	9	2	12
22	19	27	5	1	26

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