Recent Developments in xia2

Strubi early 2012 update

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Diamond Light Source

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Overview

- CCP4 2012 presentation
- Removal of frame count limitations
- Current state of multi-crystal analysis
- Other developments
- Conclusions & plans

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Removal of frame count limitations

- Use Aimless in place of Scala
- Use Pointless in place of Reindex[1]
- Run -3daii or -3da
- No more batch limitations

[1] This is still not as efficient as it could be - but it works

Example: 20 sweeps from insulin

- Insulin test sample from I04-1
- 20 sweeps: 0.2 degree / frame x 900: 18000 images
- Radiation damage very likely
- Substantial variation between data sets
- Processing rather time consuming, use a big workstation

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High resolution limit	1.66	7.43	1.66
Low resolution limit	55.18	55.18	1.70
Completeness	100.0	99.9	100.0
Multiplicity	314.3	346.7	262.8
I/sigma	81.7	228.5	7.6
Rmerge	0.106	0.071	5.227
Rmeas(I)	0.106	0.071	5.240
Rmeas(I+/-)	0.106	0.071	5.247
Rpim(I)	0.006	0.004	0.322
Rpim(I+/-)	0.008	0.005	0.450
Wilson B factor	31.457		
Total observations	2982419	44723	180512
Total unique	9488	129	687

Effects of Running Aimless

- Output effectively the same as Scala
- SD correction slightly more effective
- C++ not Fortran - no need to recompile for lots of batches
- Parallel (openMP) version in development

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Effects of Running Aimless in xia2

- Since scaling performed by XSCALE very little difference in results

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Current state of multi-crystal analysis

- Developed over 1 year or so
- Hiatus for most of that time
- Still very rough around the edges
- Requires use of XDS processing
- Requires R (at the moment) to generate plot

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Basic principles

- Assume in processing that everything comes from the same crystal
- Try to assemble a data set from everything
- Worry about isomorphism in scaling rather than from unit cell etc.
- Look at CC's between sweeps as measure of isomorphism
- Scale CC's to ersatz distance as $d = \frac{1}{CC} - 1$[2]

[2] Which means you can *interpret* the distances.

Basic Usage

```
xia2 -3daii /here/are/my/data
```

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Time passes... let's talk about options

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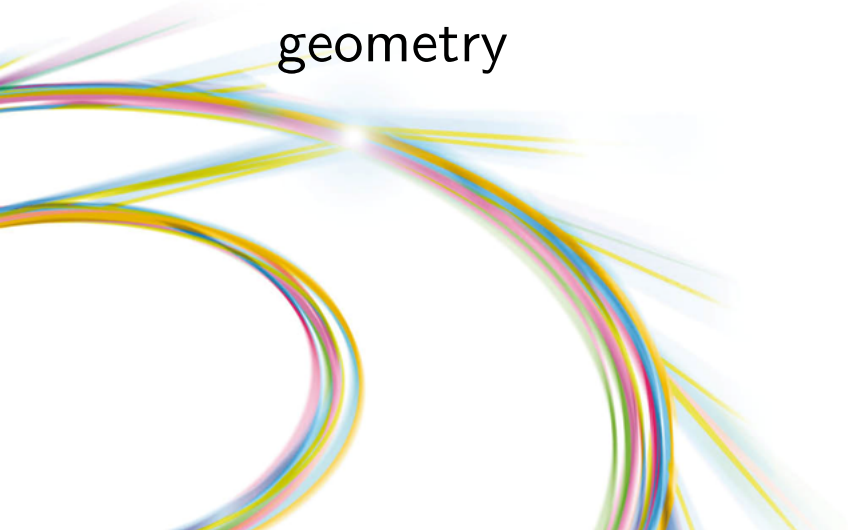
Useful options

- -microcrystal - switch to microcrystal mode
- -failover - ignore failure of processing individual sweeps
- -spacegroup - set the spacegroup as e.g. P23
- -cell $a, b, c, \alpha, \beta, \gamma$ - needs -spacegroup
- -min_images 3 - minimum images to count as a sweep
- -xparm GXPARM.XDS - refined model of experimental geometry



After processing

```
> cd DEFAULT/scale
> x1335 XSCALE.LP
> R --no-save < x1335.R
```

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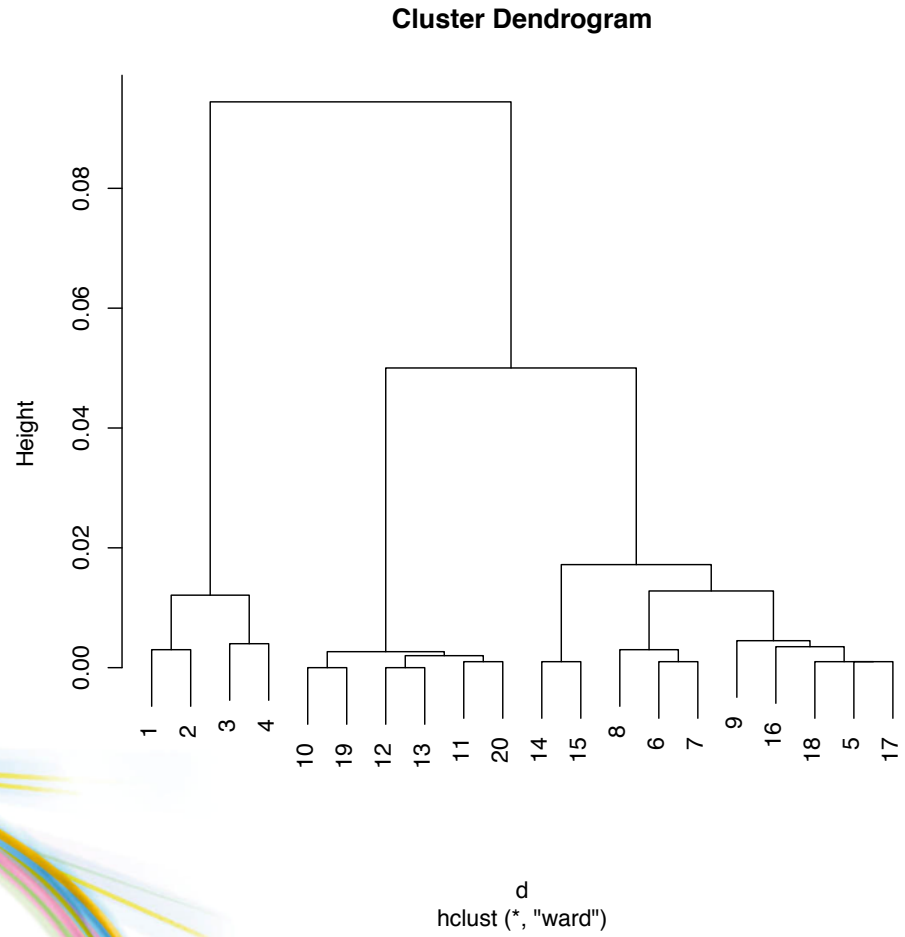
Results


Cluster Dendrogram
Height
0.00
0.02
0.04
0.06
0.08
1
2
3
4
10
19
12
13
11
20
14
15
8
6
7
9
16
18
5
17
d
hclust (*, "ward")

```
 No.   Av. CC   I/sig  File Name
   1   0.9796    2.25 NATIVE_SWEEP11.HKL
   2   0.9822    3.61 NATIVE_SWEEP22.HKL
   3   0.9807    7.49 NATIVE_SWEEP33.HKL
<snip>
  18   0.9925    2.64 NATIVE_SWEEP9.HKL
  19   0.9930    1.69 NATIVE_SWEEP10.HKL
  20   0.9826    3.39 NATIVE_SWEEP12.HKL
```

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Interpretation

- $d = \frac{1}{CC} - 1$
- $CC = \frac{1}{d+1}$
- $CC = 0.95 \rightarrow d < 0.05$
- Up to you to decide on your limits... at least you know what they mean

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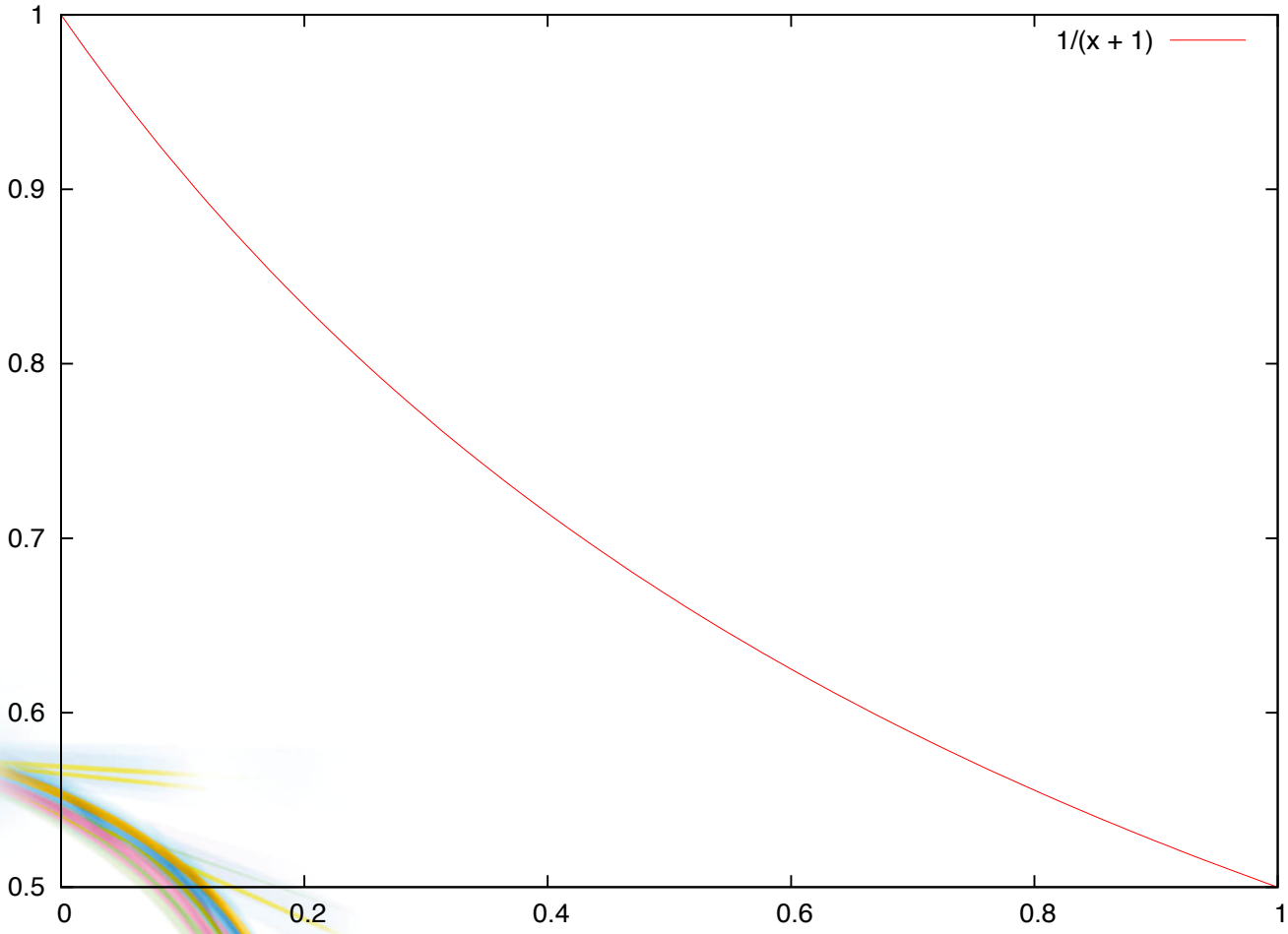
Interpretation



Next steps

- Book keeping - take the sweeps you wish to merge from dendogram
- Edit xinfo file
- Run again
- This needs automating, and also calculations performing to tell you how complete results will be

Trivial example - Thaumatin

- Split 450 image Thaumatin data set into 5 x 90 image chunks
- Process as usual, very good results and grouping comes in data collection order
- Distances are fantastically small indicating very high CC's

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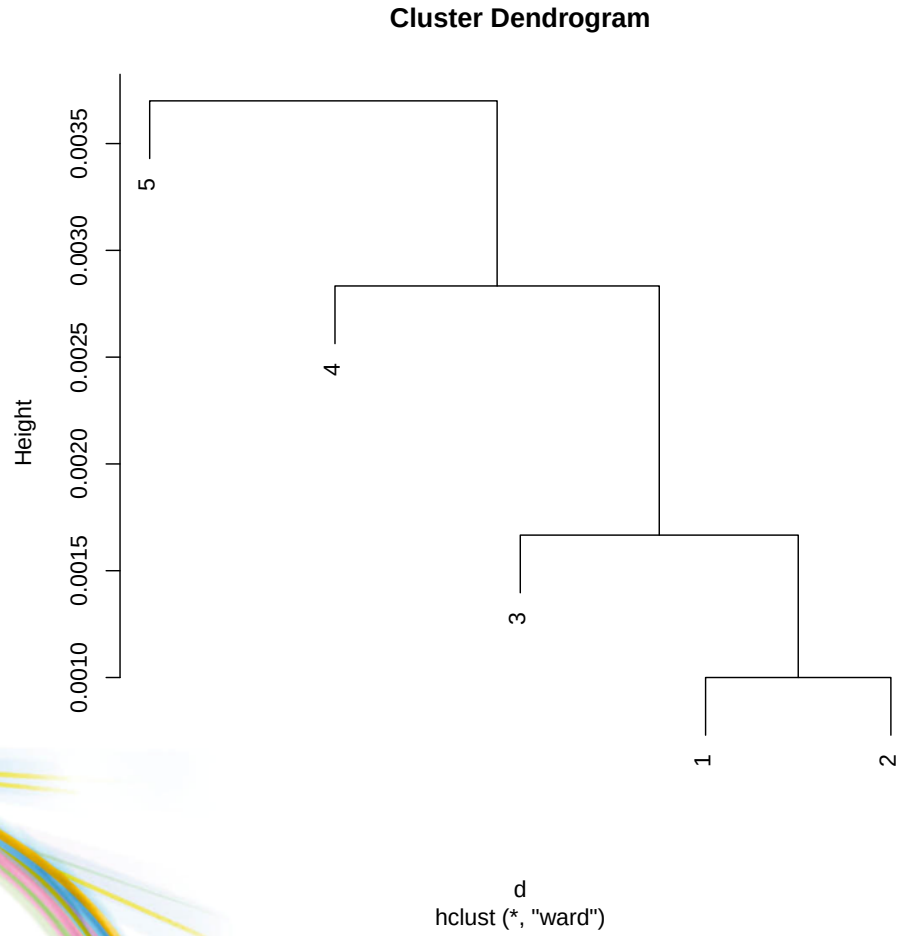
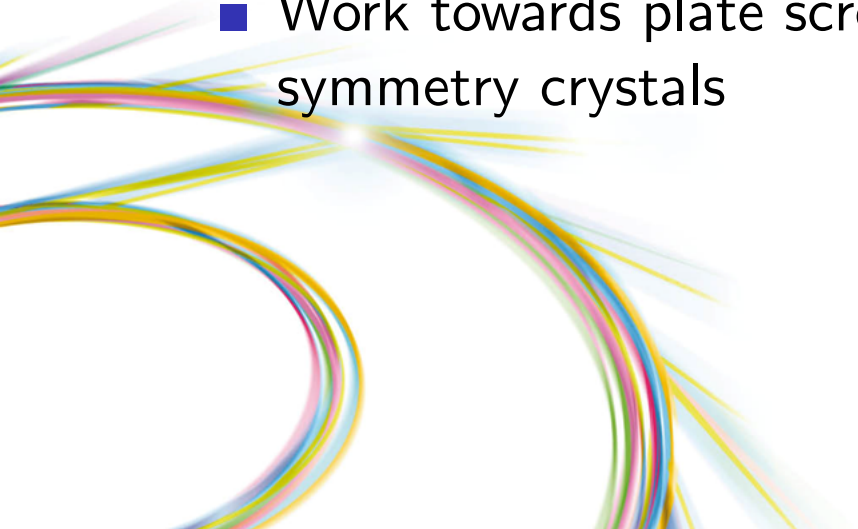
Results


Cluster Dendrogram
Height
0.0010
0.0015
0.0020
0.0025
0.0030
0.0035
5
4
3
1
2
d
hclust (*, "ward")

Developments planned from mid April

- Apply to more cases
- Work on clustering
- Include comparison of R_{merge} as a function of batch number
- Work on incorporating radiation damage: split sweeps into blocks
- Automate analysis, also allowing for completeness
- Work towards plate screening data, ideally from lower symmetry crystals



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Other developments

- Development of xia2 for small molecule crystallography
- Support for complex experimental geometry from imgCIF data
- Full scaling model search with scaling with Aimless and Scala
- Started using Phenix PHIL for parameter setting, will allow much finer grained control - any requests?

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Summary

- Support now added for much more substantial experiments, no recompile scala
- Developments ongoing shortly for properly tackling multi-crystal data analysis, particularly from plates - ideas welcome

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