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
- 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

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

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Basic Usage

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

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Time passes...

Useful options

- -microcrystal ...
- -failover ...
- -spacegroup ...
- -cell ...

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