1 Implementation of Data Processing with XDS

1.1 Introduction

This document describes the implementation of the xia2 data processing interfaces (indexing, integration and scaling) with XDS. There are two possibilities for this:

- Processing with only XDS, XSCALE - that is, not assuming that pointless, scala etc can be used.
- Processing with XDS, XSCALE and CCP4 tools - this will probably be more like the CCP4 Scaler implementation.

Perhaps there should be two implementations...?

1.2 Indexing

```
xycorr -> init -> colspot -> idxref -> [select] -> idxref
```

This will list all possible indexing solutions - the highest will be selected for integration as per the current implementation with Mosflm.

1.3 Integration 1

```
defpix -> integrate [-> correct]
```

This may recycle if the integration fails... for instance, I need to see how the TS01 NATIVE is handled by XDS integrating in oI, when mC is correct.

1.4 Pointgroup Determination

```
integrate.hkl -> combat -> pointless -> [select indexing solution]
```

This once again needs to be linked in to the indexer as per the CCP4 Scaler implementation.

1.5 Integration 2

```
[select indexing solution] -> defpix -> integrate -> correct [in correct pg]
if fail, --spacegroup; repeat
```

This may work out as being the same module as Integration 1, if it is implemented in the same way as the CCP4 system.

1.6 Reindexing & Spacegroup Determination

```
[sweep 1] -> [quick scale]
[n] * xds_ascii.hkl -> pointless [reindex against quick scale] -> correct
```

1.7 Scaling & Merging

```
xscale [output unmerged] -> scala
```