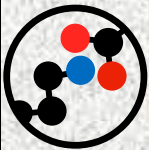

Pilatus Data Processing at IMCA-CAT

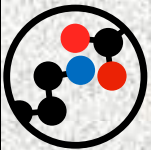
**Kevin Battaile
IMCA-CAT**

Hauptman-Woodward Medical Research Institute



Introduction

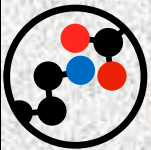
- General requirements.
- Available options.
- Hardware implementation.
- Default work flow.



General Requirements

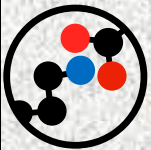
We have a consistent user base with (relatively) well-characterized projects.

- Fast data processing.
- Must be able to run unattended.
- Must be reliable / robust.



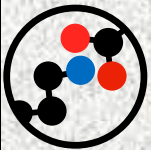
Available Options

- Processing Software
 - XDS
 - MOSFLM
 - d*TREK
- Wrappers
 - autoPROC
 - ELVES
 - XDSAPP
 - xia2
 - ???



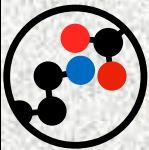
Available Options, 2

- Requirements
 - Scriptable to run unattended.
 - Speed
 - XDS only multiprocessor-compatible software
 - Not reinvent the wheel, if possible.
- Conclusion
 - All IMCA members are Global Phasing consortium members, so autoPROC was chosen as the package to use.



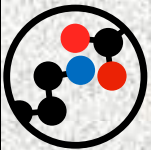
autoPROC: what is it?

- Wrapper for data processing software.
- Can use XDS or MOSFLM for integration.
- Uses Pointless for SG identification.
- Uses SCALA for scaling.
- As simple as typing 'process' in your images directory.



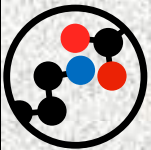
Implementation

- 16 core processing server.
 - Takes advantage of XDS' MP capability.
 - Enough CPU power for concurrent users.
- SCALA is still the bottleneck in the process as it is not MP capable.
- Users can log in remotely at any time.



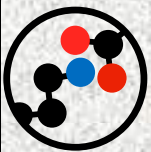
autoPROC Default Work Flow

- Spot search on all images.
- Index
- Integrate in P1 despite indexing result.
 - Will integrate in a provided SG/unit cell.
- Pointless determines / refines SG params.
- Rerun integration with refined SG params.
- Pointless converts XDS output to mtz.



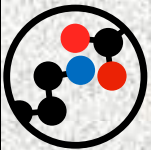
autoPROC Work Flow, 2

- Iteratively run SCALA until a variety of preset scaling requirements are met.
- Output scalepack file.
- Run Truncate then Unique to output mtz file with free reflections.
- Scaling module can be run independently.
- XDS keywords can be included on command line and other options included to control scaling behavior.



Usage

- Most people run from the command line.
- Some groups have a script that will automatically run with specific options.
- Potential future work could involve creating a pipeline to automatically run autoPROC against a collection directory.



La Fin

- autoPROC
 - <http://www.globalphasing.com/autoproc>
 - Vonrhein et al., (2011) Acta Cryst D67:293
- IMCA-CAT
 - Lisa Keefe
 - Anne Mulichak
 - Kevin Battaile
 - Eric Zoellner
 - Lewis Muir
 - Joe Digilio

