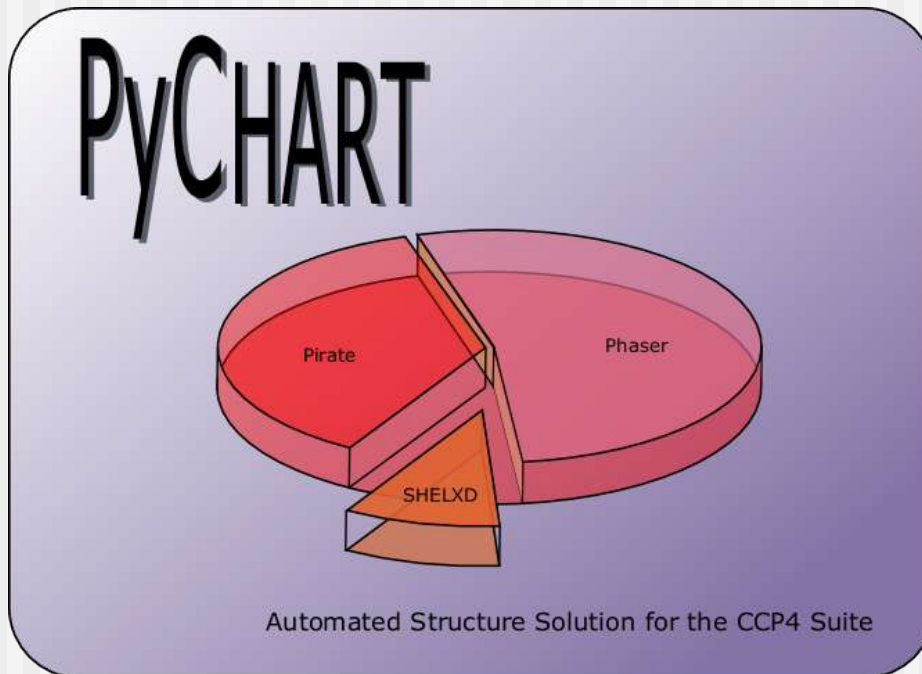
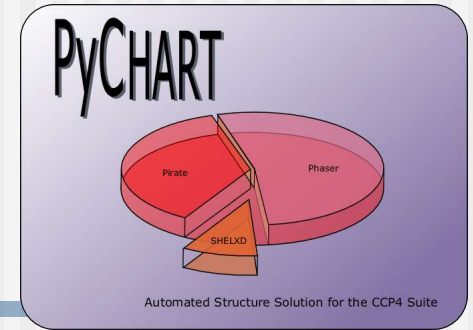


PyChart (the future)

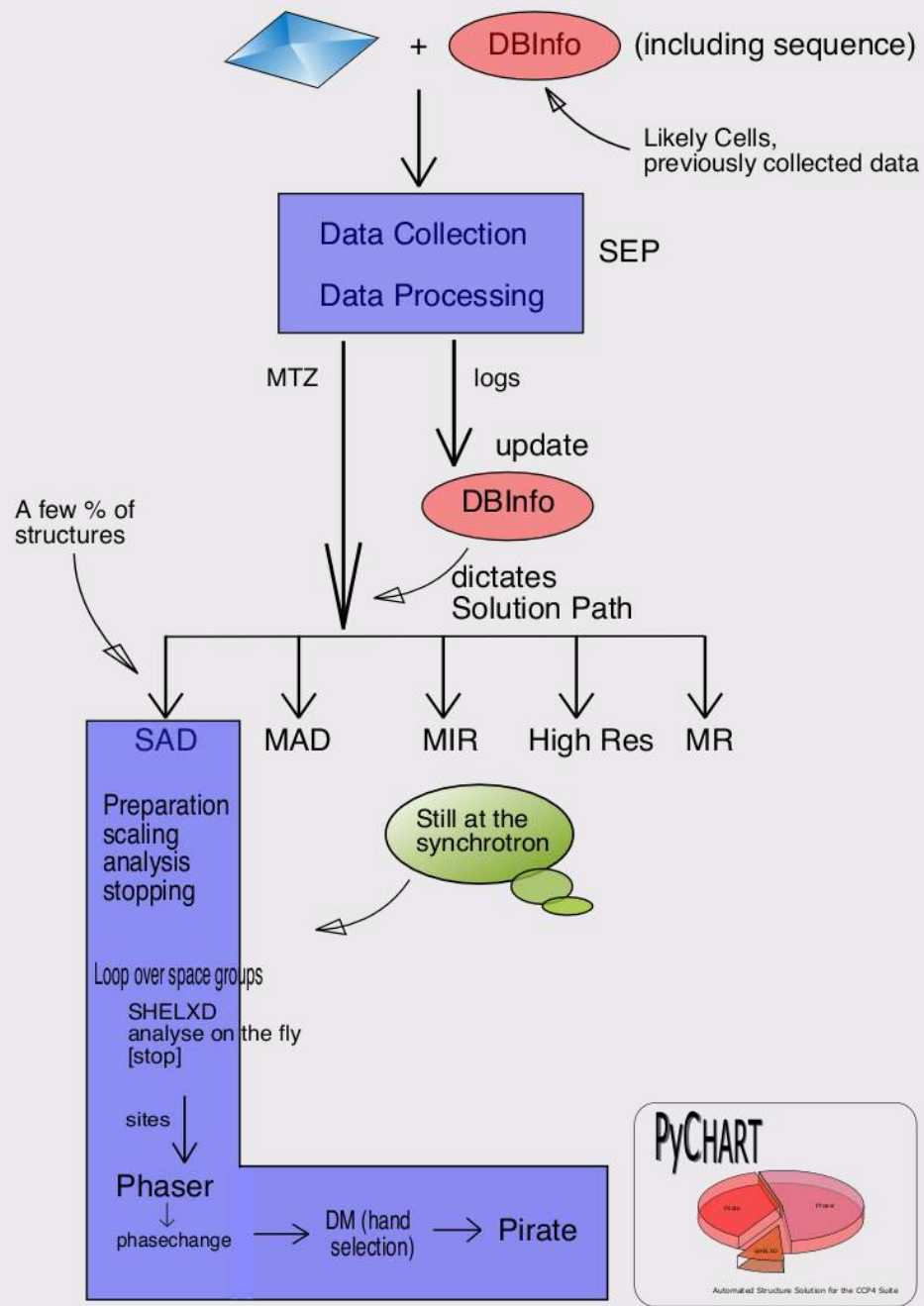


PE & DR

PyChart version 1.0



- Presumes de-twinned, Laue group known, consistently indexed
- Uses scaleit, ccp4 utils, SHELXD, Phaser, DM, Pirate
 - And connectivity program from Clipper/Coot?
- Result: An interpretable map



PyChart Version 1.0

PyChart Version 2.0(?)

- As above with:
 - Consistent indexing correction
 - MAD and MIR(AS)?
 - Buccaneer or other tracing program
 - Including sequence assignment
 - (Re)Building functions from Coot?
 - Recycling?
 - Protein model improves HA model?

Cross-talk thoughts

- MAD and MR structure solutions can interact
 - e.g. low homology model + Zn Anomalous
 - Get Poor map from experimental phasing with anom
 - Position molecule (FFFear/Molrep)
 - Refine/Rebuild using exptl. phases

Gaps in PyChart

- Analysis/Correction of Indexing/Twinning
- MAD and MIRAS
- Map skeletonizability and/or variance variance analysis
- Sequence assignment
- Model-building

Gaps in Ligand Fitting Pipeline

- Everything except (perhaps) the ligand searching
- Coot has “automated” rotamer optimization
 - Needs to be moved out of graphics
- Model combination, ligand orientation, post-refinement, validation
 - All TODO

Current Tools in Coot...

...useful in a automation system

- Terminal residue addition/loop fitting
- Residue range zeroing
- Validation
 - Residue density fit, temperature factor analysis - available command-line progs with XML output
- High Res model-building