

DIALS Project Update

MRC LMB update 22nd May 2013

Overview

- Project philosophy
- Project plans
- Team responsibilities
- Other things ongoing at Diamond

Project Philosophy

- We cannot design this right from the outset
- We cannot do better than existing programs without first doing as well as them
- We cannot do as well as everyone else without first making a simple program that works
- We don't know which methods are "best" so design in all from the start
- Also make it simple to add new ideas in the future

Project Plan & Timeline (Integration)

End April - Finish centroid methods, work out joint API

End May - Simple 2D and 3D summation integration, requires:

- unified background determination probably using two methods (shared API)
- reflection data management method
- unified shoebox handling
- full refined model (may need to apply some additional local refinement to make this work by this deadline)

Project Plan & Timeline (Integration)

Mid June - Unified API for summation
integration methods as well as possible

End August - 2D and 3D profile fitting methods
sharing / extending existing API for
summation

integration sharing common code structures
where possible

Stretch goal: recycle centroids calculated from
the integration into model refinement

Project Plan & Timeline (Refinement)

Ongoing in parallel with integration efforts:

- time dependent modelling (end of June)
- integration of time dependent model with integration software (July)
- improved refinement methods (e.g. SVD etc. around end Aug)

Team Responsibilities

- David Waterman - refinement
- James Parkhurst - 3D methods and dxtbx
- Luis Fuentes-Montero - 2D methods and peak modelling
- Graeme Winter - coordination and integration with xia2, day-to-day project management
- Gwyndaf Evans - project leader

Related Projects (at Diamond)

- X-FEL data analysis following Strubi visit to LCLS - primarily Graeme with LBL team
- Multi-crystal data analysis PDRA