

DIMPLE - The joint DLS/CCP4 Difference Map Pipeline

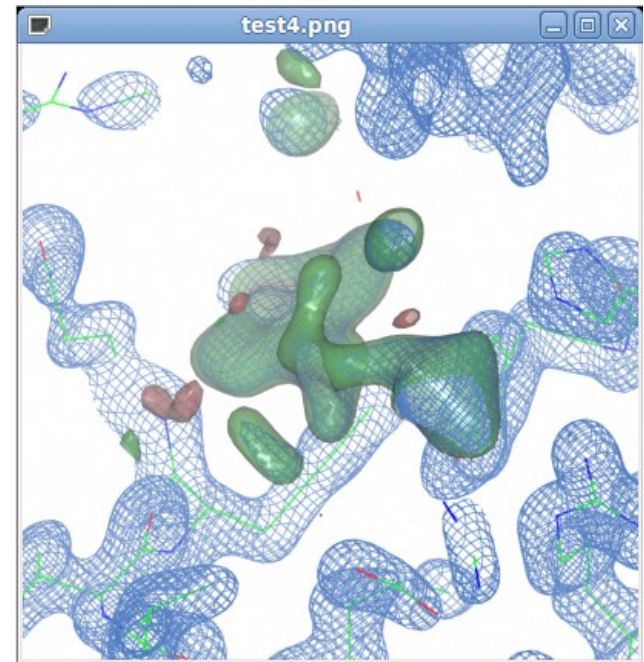
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Overview

- Automated difference map generation pipeline to allow for quick assessment of crystal data to see if a ligand has bound to the structure
- EDNA implementation of the solve-o-matic pipeline already in use at Diamond (original script by Dave Brown) with some extra functionality
- Project adopted by CCP4 as part of the CCP4/Diamond MX collaboration initiative
- To be deployed at Diamond and distributed as part of the CCP4 suite

Goal of DIMPLE

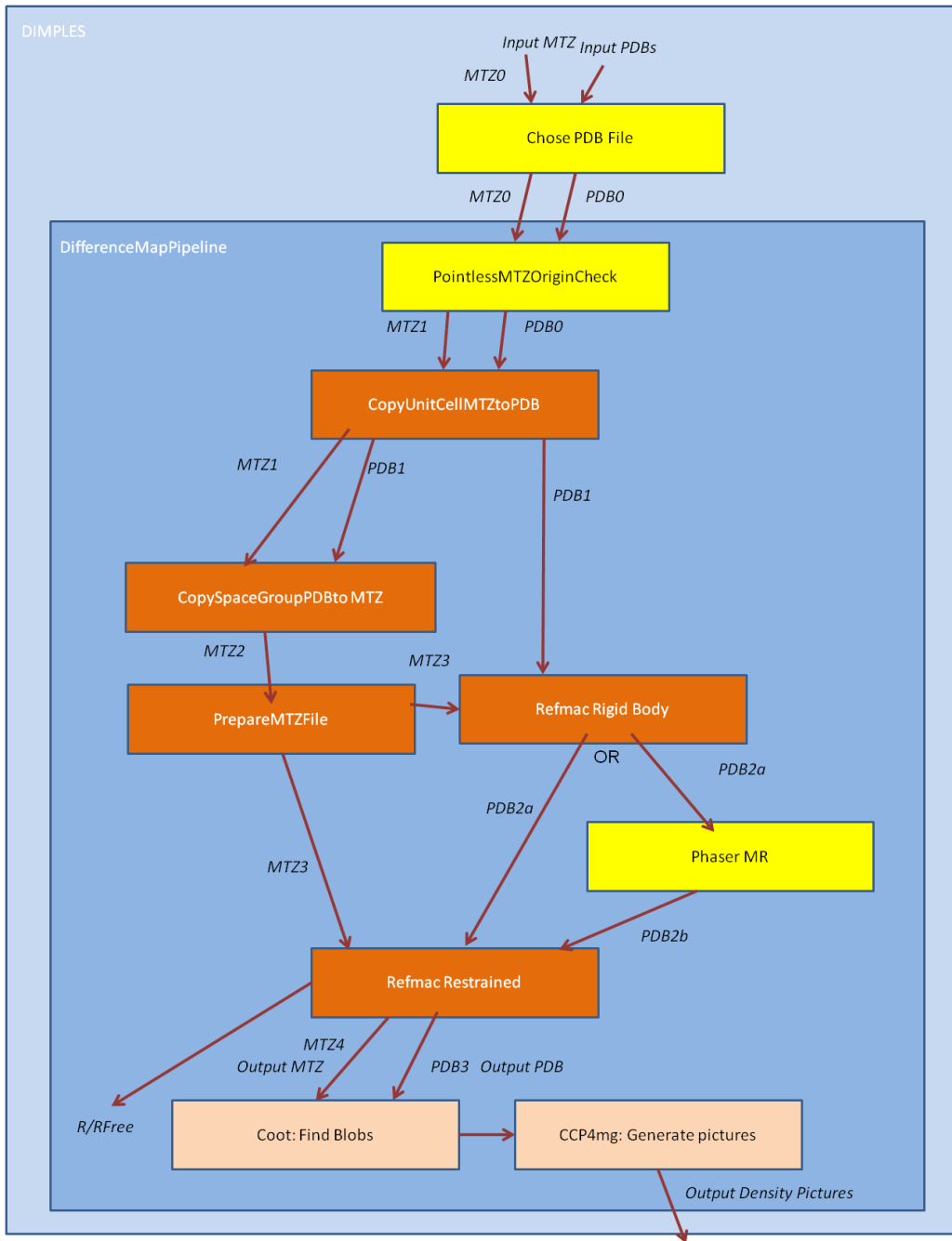
- To make the process of screening crystals for bound ligands quick and efficient
 - Go from merged MTZ file to refined density map automatically and in a short space of time
 - Present the user with set of images of the interesting, pieces of density in the difference map
 - Allow the user to quickly decide if the crystal has a bound ligand present or not



EDNAfication

- Built upon a first layer of Exec Plugins to perform individual CCP4 application tasks
 - Getting space group information from MTZ files using Mtzdump
 - Doing rigid body refinement with Refmac
- Related Exec Plugins are grouped together into second layer of Control plugins
 - Copying unit cell information from an MTZ file to a PDB file
 - Preparing an MTZ file for Refinement
- A top level Control plugin wraps around the basic control plugins to control the overall pipeline

DIMPLE pipeline plugin layout



Experience of using EDNA

- Advantages:
 - Common framework makes collaboration on a project work well
 - Strict guidelines as to how to develop plugins makes it easy for novice developer to design and create plugins
 - Good community support
 - Modularised approach allows for re-usable components
 - Comprehensive testing framework

Experience of using EDNA

- Disadvantages:
 - Steep learning curve
 - Use of UML modelling can add a lot of overhead time to the development
 - Reliance on Enterprise Architect
 - Limited documentation (but this has improved)
 - Windows support

EDNA and CCP4

- Perception within CCP4 is that EDNA is a good framework for developing automation pipelines and in our efforts to collaborate with Diamond, ESRF and other synchrotrons we should use it
 - DIMPLE
 - Balbes
 - MrBUMP/Buccaneer pipeline
- It was felt that as a general purpose framework for CCP4 it wasn't the correct tool
 - Not designed to provide the level of interactivity required by CCP4
 - Too difficult to get our dispersed community of developers to adopt it
 - A lighter framework specific to CCP4's needs would be developed

Acknowledgements

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