

Experimental Phasing Overview

CCP4 Developers Meeting 2007

March 27, 2007

Integrating Many Major Parts For Best Phasing

- “Experimental Phasing” can no longer be viewed as a discrete entity
 - *e.g.* Refmac + SAD function for heavy atom substructure refinement
 - * Considerably improves the amount of buildable structure

HAPPy

Tools for the SAD job

- with Phaser, BP3, SHELXD, pirate
 - Top class tools
 - Buccaneer: still in development
 - * unproven

HAPPy

- The CCP4 Experimental Phasing Pipeline “Framework”
 - Using data from TRUNCATE/U-BOAT
 - Task 1 (Release 1.0)
 - * Obtain an interpretable map
 - * SAD only
 - * CCP4i interface required

What are we trying to achieve?

- 2 regimes:
 - Fast
 - * While on the beam line:
 - “Can I solve my structure with these data?”
 - Rigorous
 - * While back home:
 - “Make me the best phases and model”

Current Status

- Take input via XML Project file and MTZs
 - Prepare and analyse data
 - Determine resolution limits
 - Anomalous difference limits
 - For each possible space group:
 - For each set of resolution limits
 - * Determine heavy atom sites (SHELXD)
Select solution with best CC score from SHELXD For each phasing program (in Phaser, mlphare, BP3)
 - * Phase each substructure hand
 - Useful if Phaser made “inverted hand” phases
 - Score phased maps using variance analysis (CFFT) Choose correct substructure hand if possible
- For each resulting phased data set: Refine with PIRATE

Things to Worry About

- Nobody other than a masochist would use CCP4 to solve their experimental structure
- Preparation of F_{AS} , anomalous data
- Integration of structure solution with database
 - We will populate database with substantial number of our (own) types of table
- CFFT variance analysis is not a good scoring system
 - Other criteria required

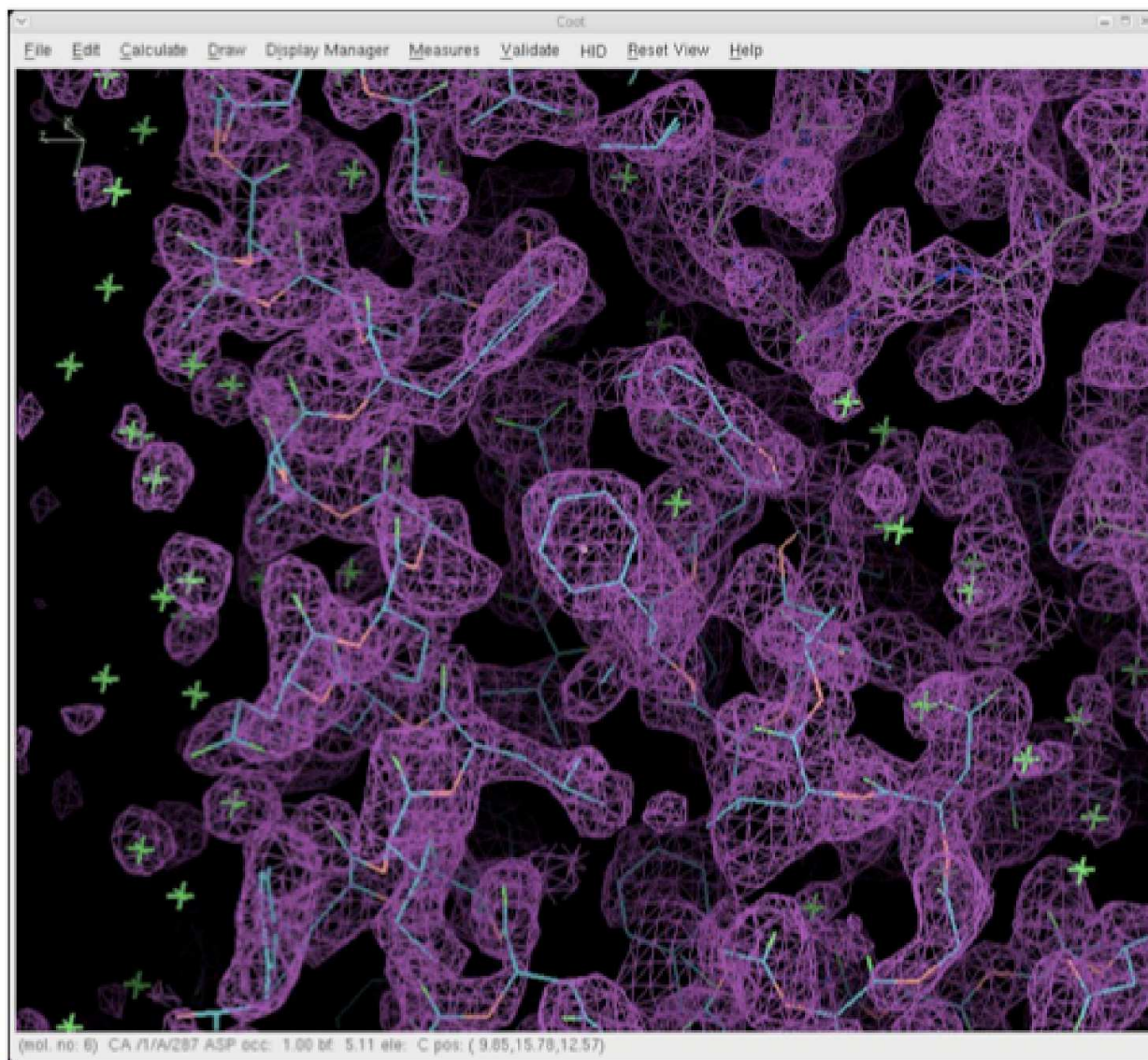
More Things to Worry About

- Need noses on the grindstone...
- Release, release!
 - We are already 6 years behind
- Packaged usefully (for users)
 - Currently in a mess
- Need a nicer GUI
 - Prototype GUI is a good start but not yet informative enough
- We'll need to do more than SAD

What are we doing right?

(What is different to CHART?)

- It uses the best tools
- It works on many data sets
 - (it is more simple than CHART)
- It is part of CCP4
 - Collaborative
- Integrated with CCP4 database
- Dan is working full-time
 - Not a week-end project



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