What's new in: Phaser

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CCP4 Study Weekend
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Phaser – new developments

Next version: 2.2.4 (2.3.0?)

General
- faster minimiser
- changes in keyword input
- map sharpening

Experimental phasing
- reassign anomalous atom type in experimental phasing
- map coefficients without real scattering contribution for density modification
- better treatment of anomalous scatterers inside partial MR models
- wavelength-dependent f' and f" restraints

Molecular replacement
- OpenMP – fast rotation function
- OpenMP – brute rotation and translation function
- OpenMP – packing and refinement
- B-factor refinement
- model error refinement
- automatic search order determination
- model symmetry
- fast mode
- analytic second derivatives
- template matching
- faster, more intelligent packing test

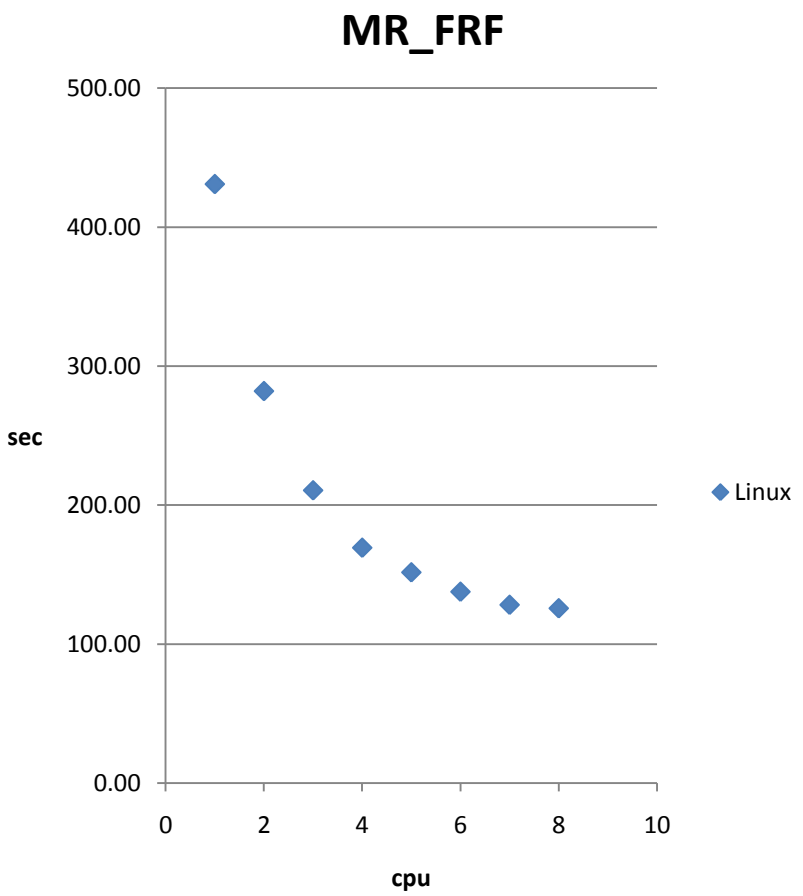
OpenMP support

- everything with a progress bar can be run in parallel

```
Spreading calculation onto 8 threads.
0%                                                  100%
|================================================| DONE
```

- controlled by JOBS keyword
  default: 1
  max ≤ number of CPUs

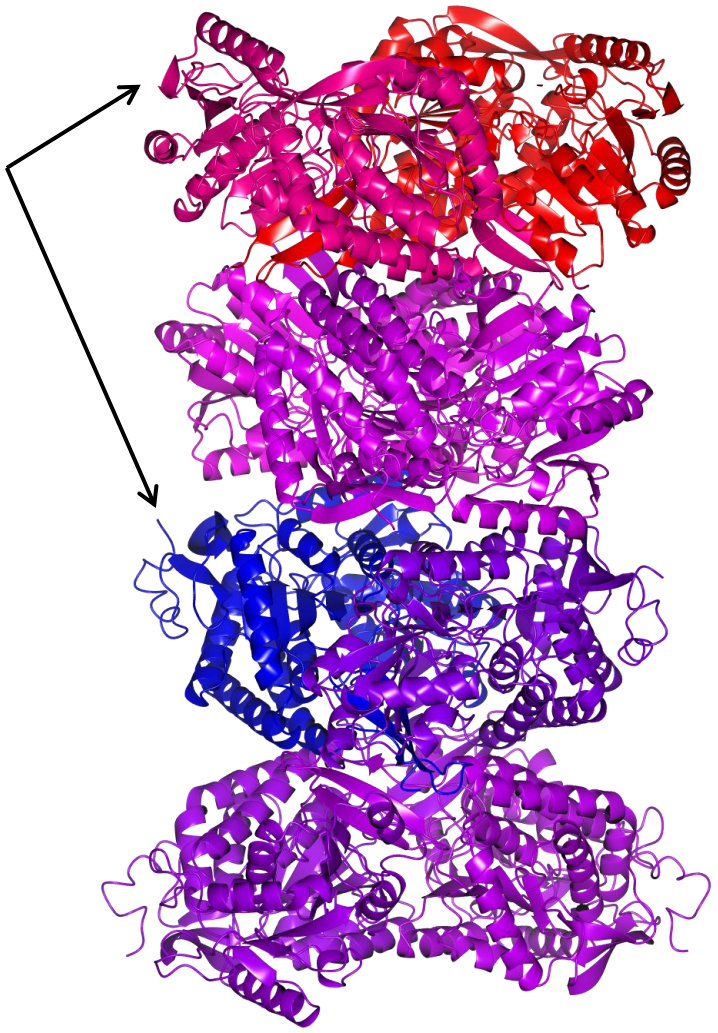
- **uses more memory!**



B-factor refinement

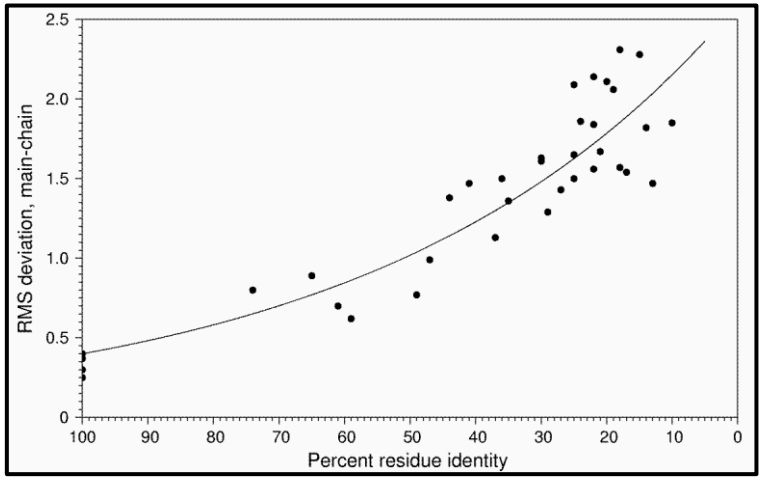
For multimer models, B-factors typically differ between chains

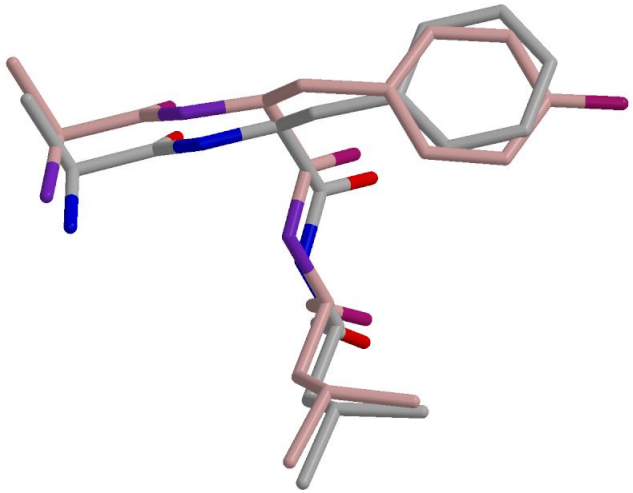
- additional chains are found by taking the present structure into account and trying to explain the difference
- refining the B-factor for a chain makes the estimate for the “missing” structure factor more accurate



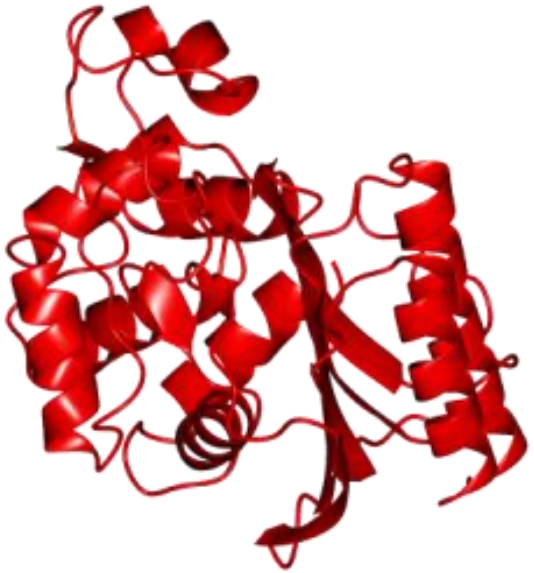
Model error refinement

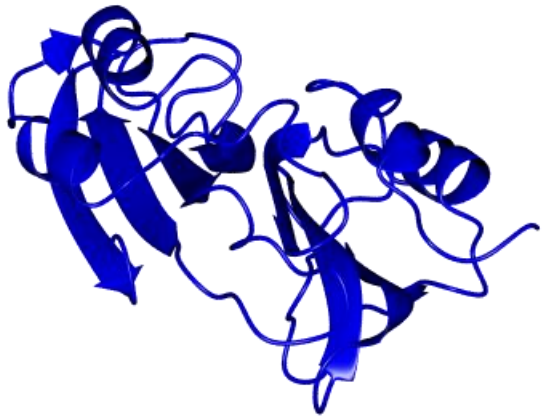
- model error is typically an estimate from sequence identity
- if a solution is found, the error can be determined more accurately
- better model error improves phases and helps locating subsequent molecules





Search order determination





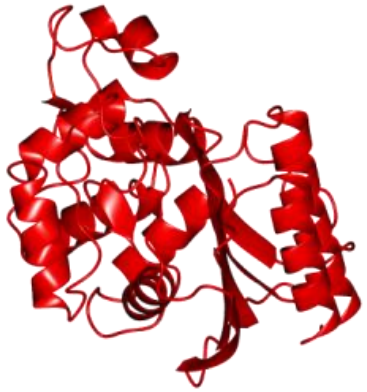
65% of structure
35% identical model

35% of structure
50% identical model

Which model is easier to find?

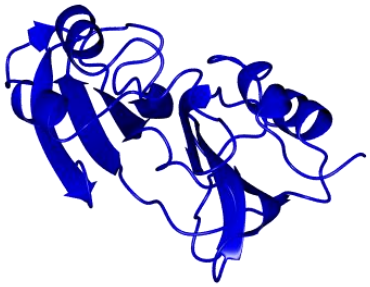
Search order determination

A better model explains more of the data



65% of structure
35% identical model

Better model if data resolution is low



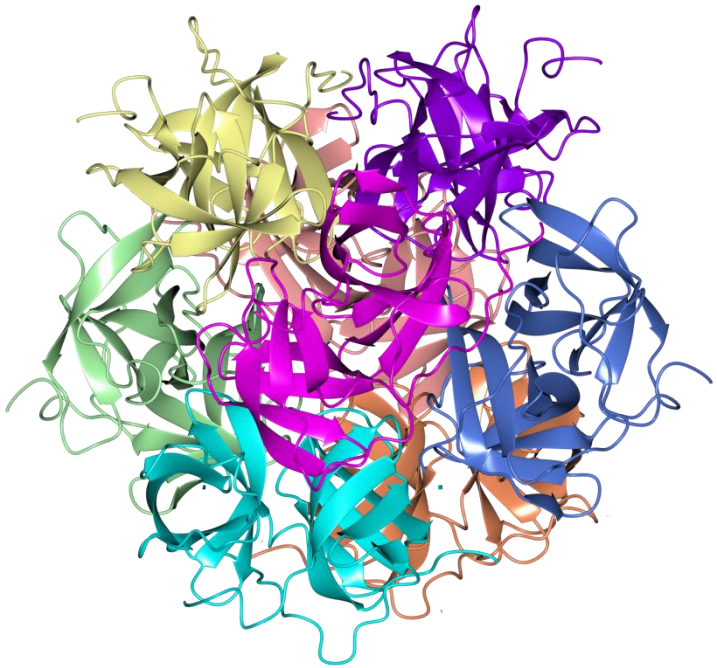
35% of structure
50% identical model

Better model if data resolution is high

Model symmetry

Model with point group symmetry

- several identical solutions
- difficulty in identifying solutions

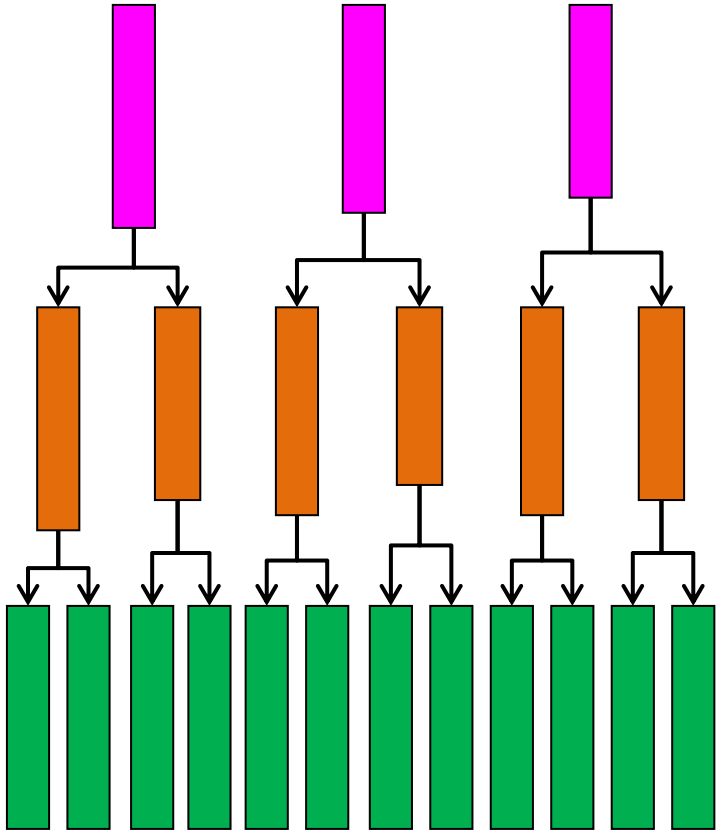


Phaser

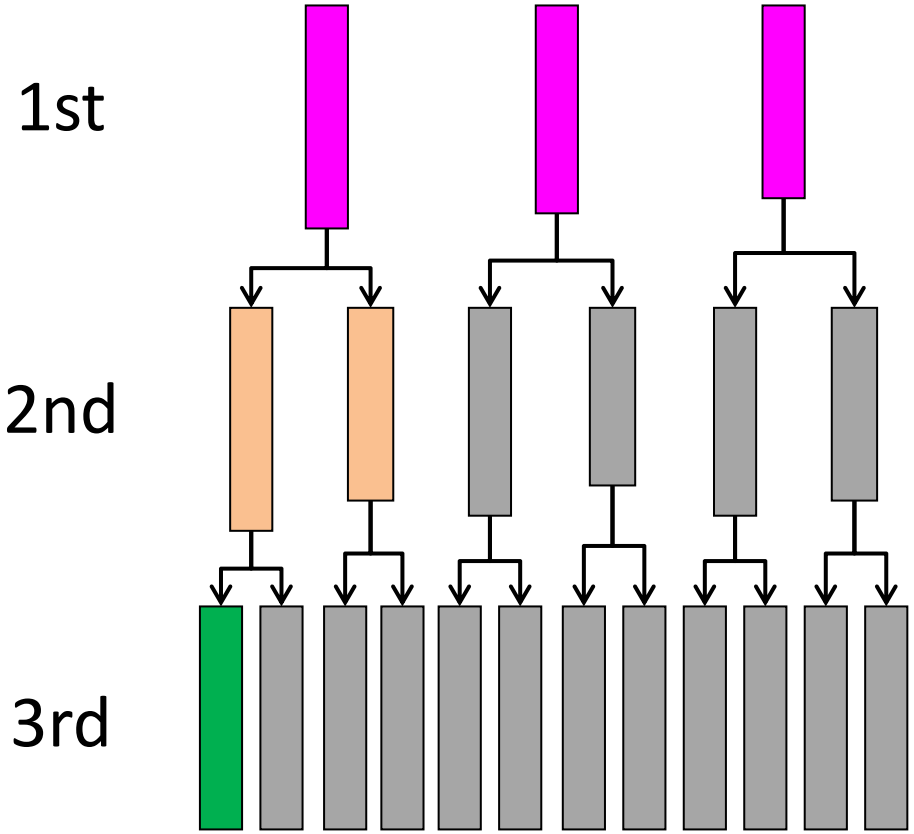
- extended solution identity determination taking internal symmetry into account
- automatic point group symmetry detection tolerating small differences between chains

Fast mode

MR_AUTO mode



MR_FAST mode



Fast mode

identify solutions (8.0 ≤ TFZ)

↓

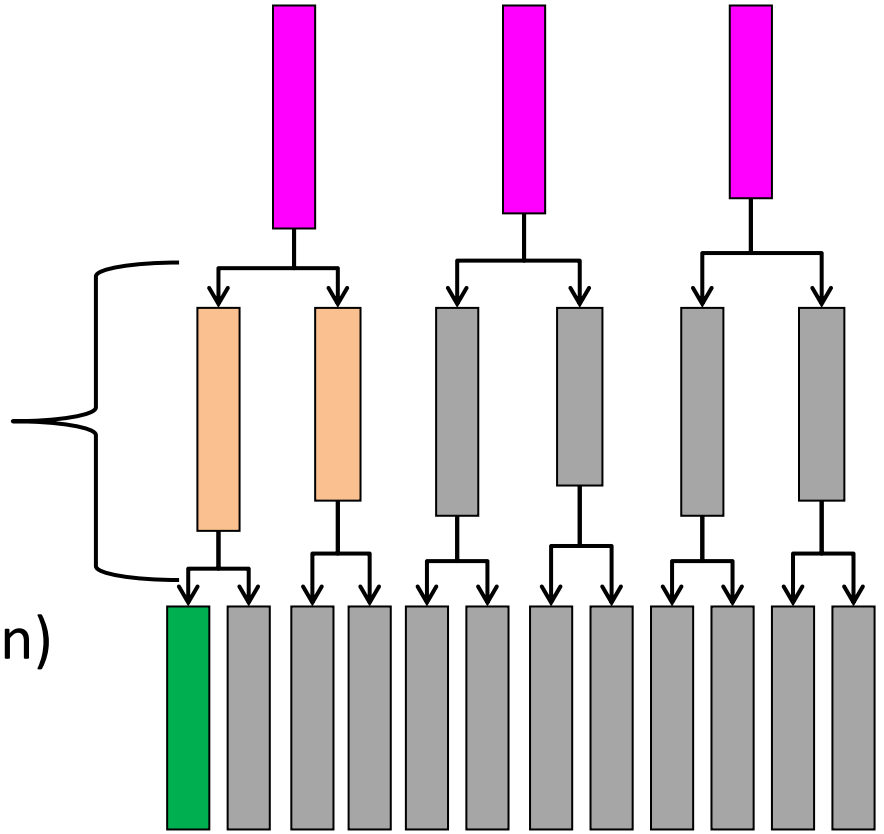
“amalgamate” independent molecules

1. discard if clashing
2. discard if LLG lower

(repeat if more than one solution)

↓

final solution



Packing test

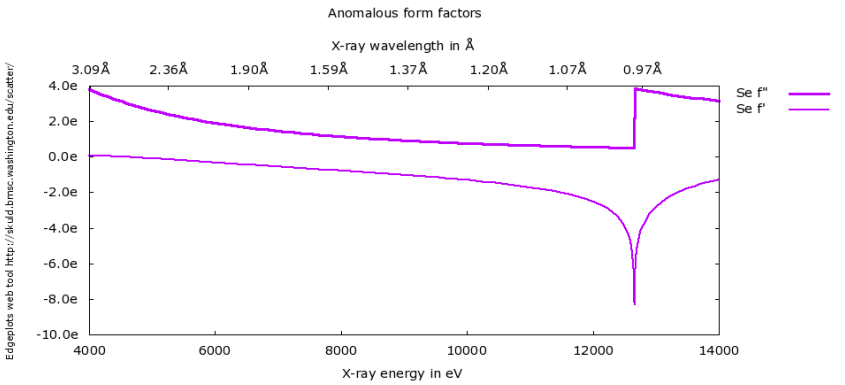
- **scale allowed clashes with structure:** specify allowed clashes as percentage
- **fast packing test:** do not count all clashes, only up to maximum allowed

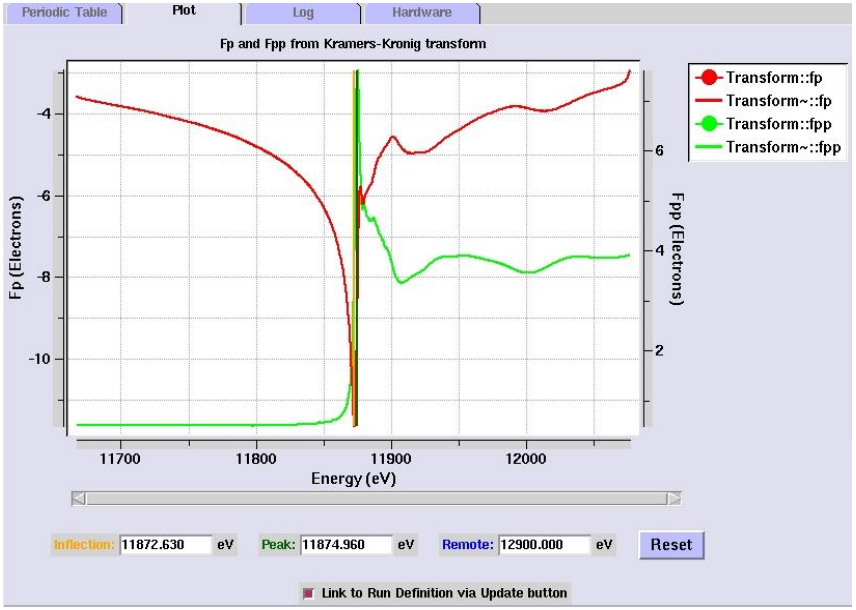
Other improvements in MR

- faster refinement (analytic second derivatives)
- ability to match solution with previously established solutions (“templates”)

f’ and f” restraints

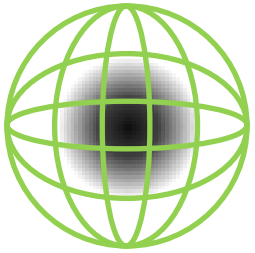
- f’ and f” are restrained to stabilize refinement (correlation with occupancy)
- tight restraints are used if not near an absorption edge
- loose restraints are used when near an edge
- **atom type** and **wavelength** now compulsory inputs



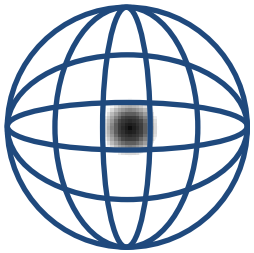


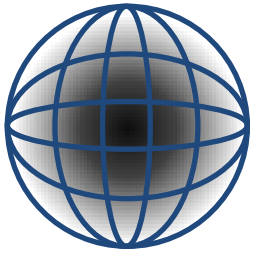
Atom type reassignment

- atom identity is guessed when site is located

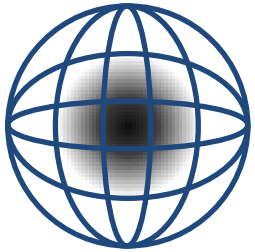


- this may turn out to be incorrect when the model improves





- checks for site identity in every cycle using site occupancy calculated assuming every possible heavy atom type

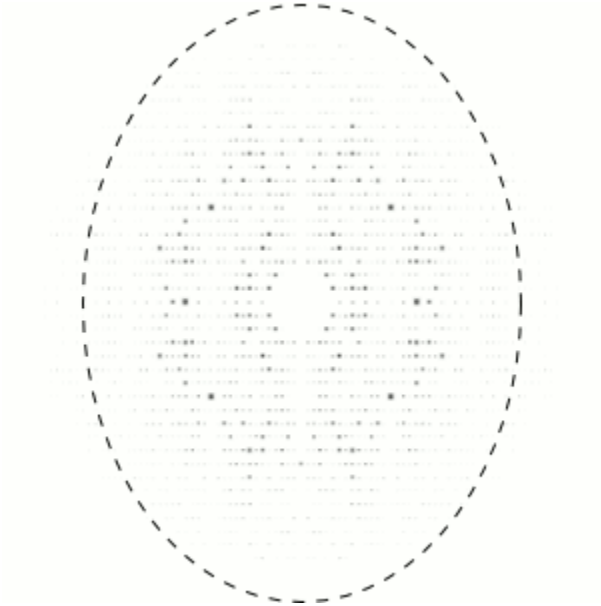


Other improvements in EP

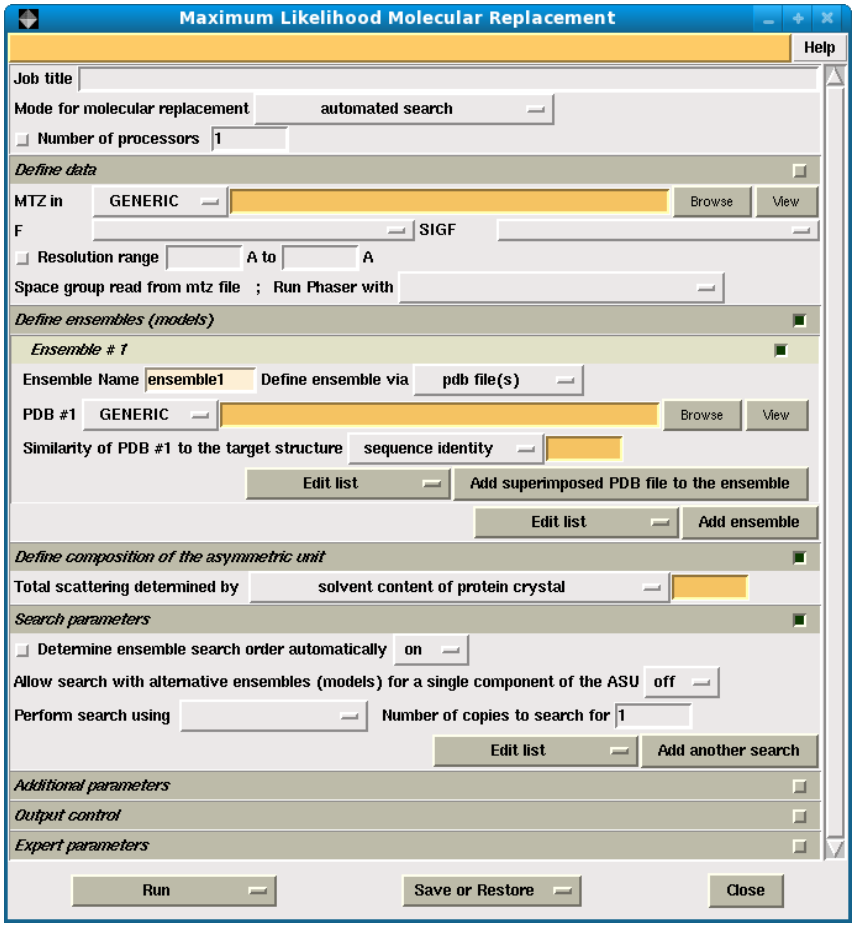
- delete only nearest atom from partial model if an anomalous atom is found inside the model
- output map coefficients without real scattering contribution (use in density modification)

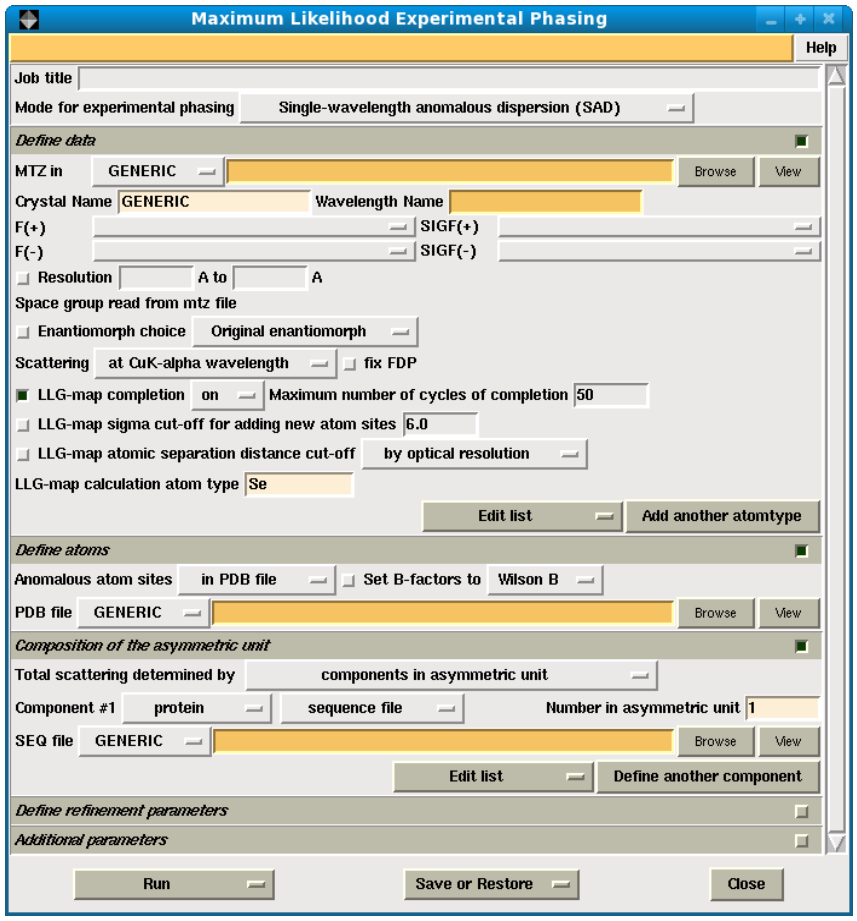
Map sharpening

- scale map coefficients according to steepest anisotropic fall-off
- visual increase in map quality



New CCP4i

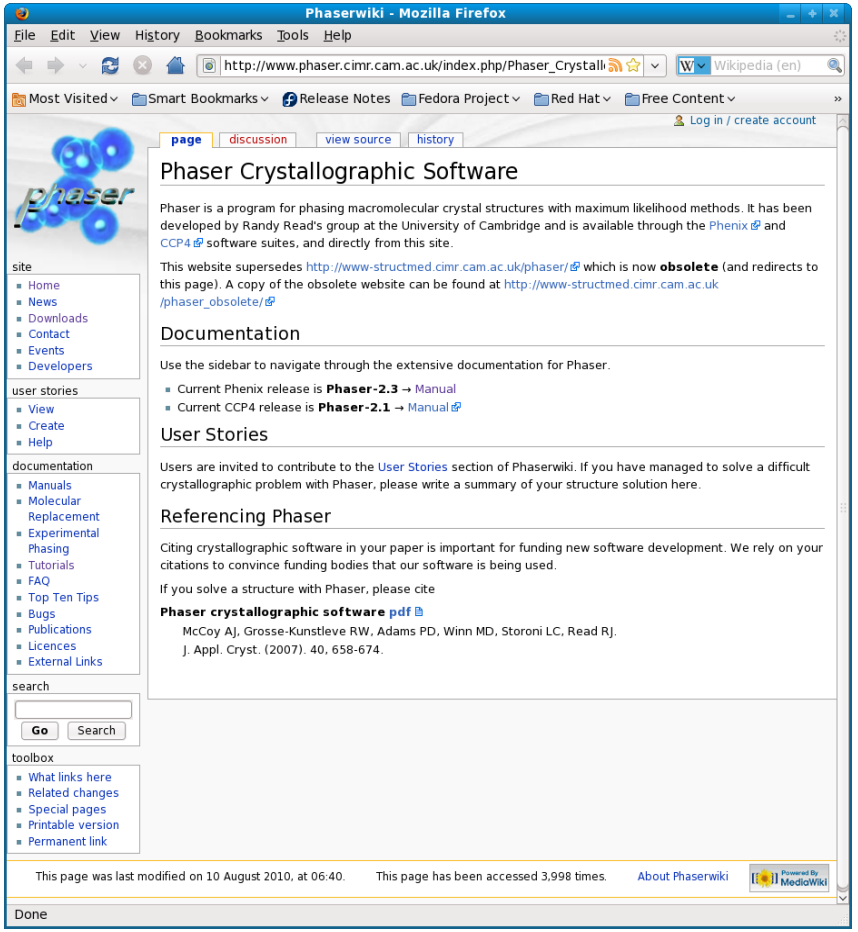




(keyword input changed, old parameter files cannot be used!)

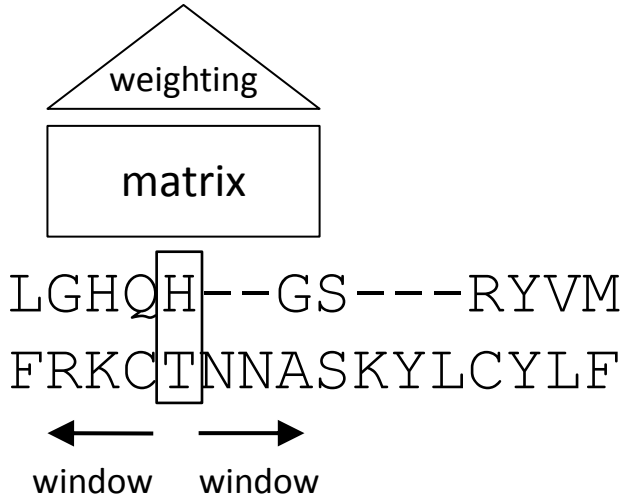
www.phaser.cimr.cam.ac.uk

- wiki format documentation (more up-to-date)
- portal to share recipes and scripts for the community
- (nightly builds distribution – coming!)



Sculptor: model improvement

- improve models using information from sequence alignment (sequence similarity)
- modifies main chain, side chain and B-factors
- pre-defined protocols to generate good model variability



sequence similarity calculation

Sculptor: model improvement

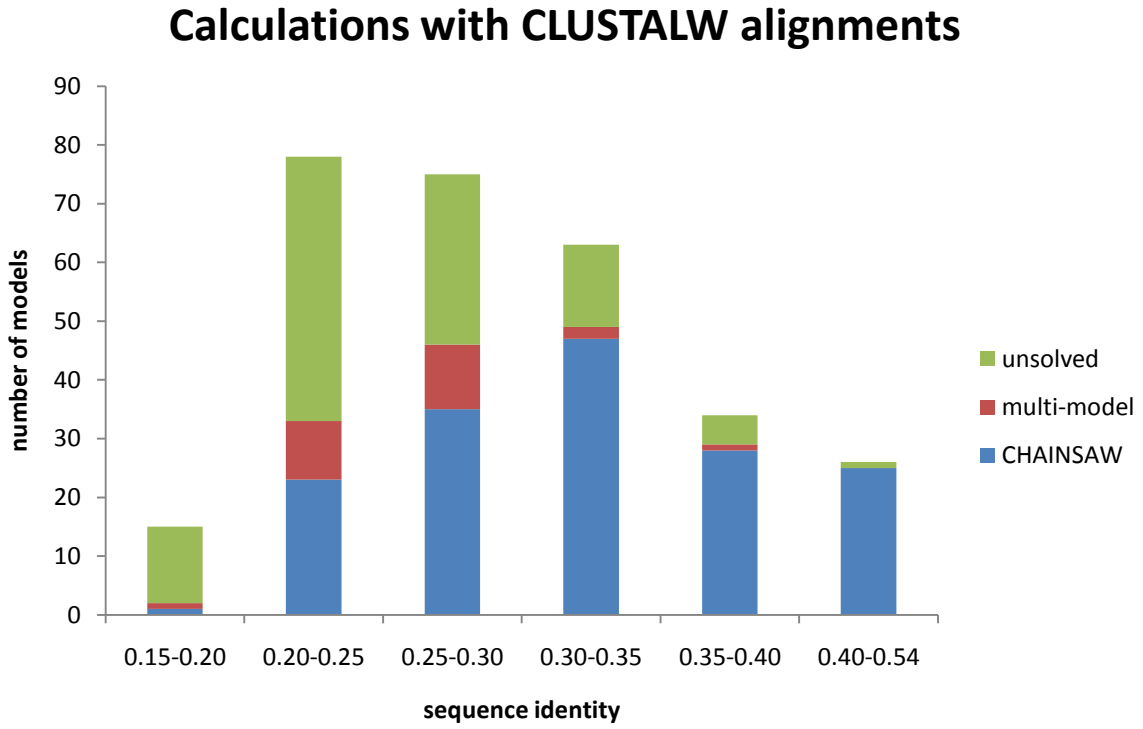
Model
CHAINSAW

Model
Sculptor

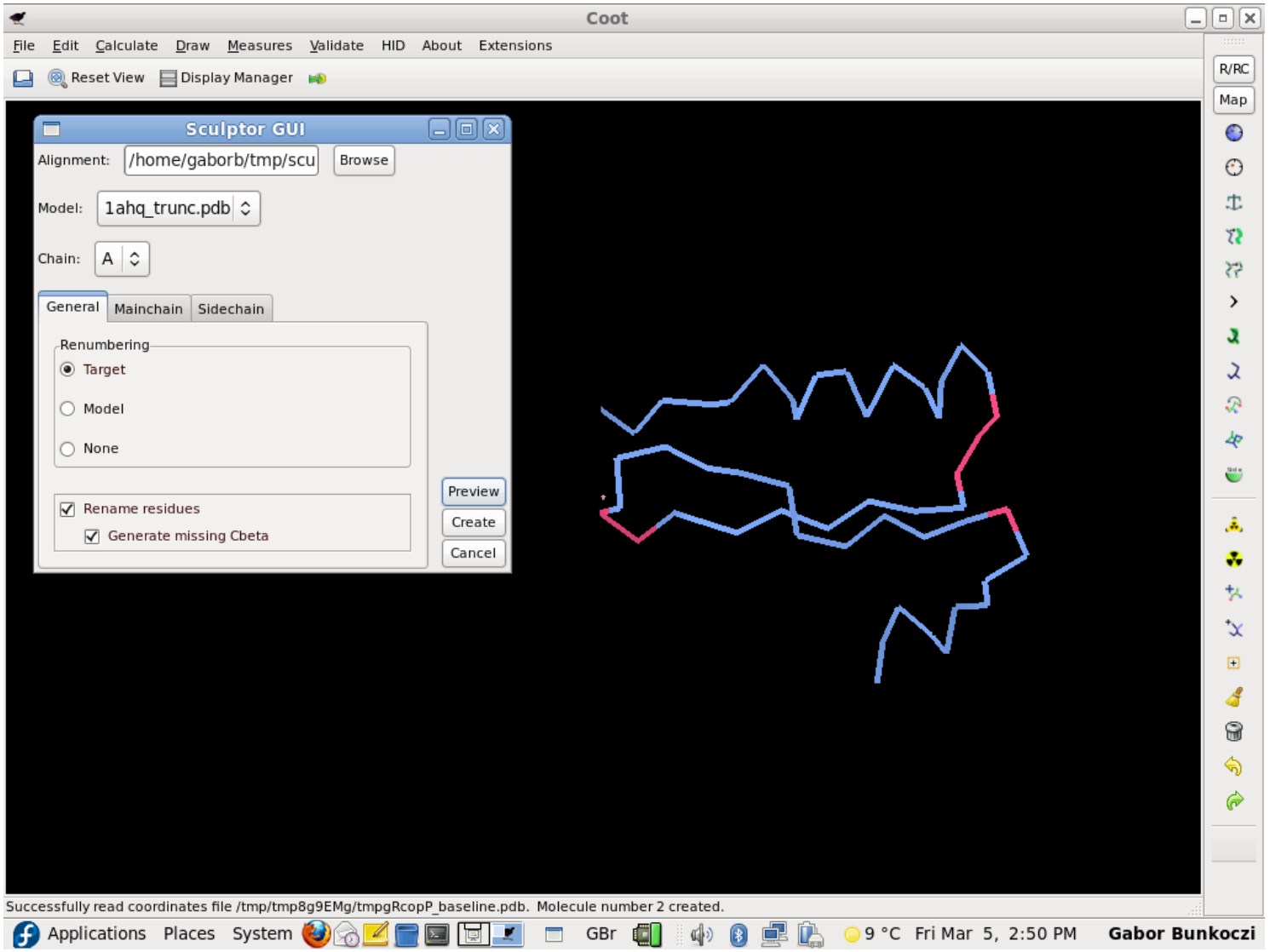
Model
Sculptor +ASA B-factors

Model
Sculptor +sequence similarity B-factors

Model
Sculptor +sequence similarity B-factors + ASA B-factors



Sculptor: interactive editing



Acknowledgements

Python-based Hierarchical Environment for Integrated Xtallography

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