

# Computational Tasks in Protein Crystallography

## Data collection

### Data processing

- Indexing
- Integration
- Scaling
- Truncation (I -> F, Wilson B-factor)

### Structure solution

- phases known: structure known, molecular replacement
- phases not known: experimental phasing

### Structure refinement

- re-set B-factor to average value
- rigid body refinement
- manual inspection of map and structure; manual adjustment
- positional (all-atom) refinement
- grouped B-factor refinement
- individual B-factor refinement
- positional (all-atom) refinement
- manual inspection of map and structure; manual adjustment
- simulated annealing
- positional (all-atom) refinement
- re-set B-factor to average value
- grouped B-factor refinement
- individual B-factor refinement
- positional (all-atom) refinement
- manual inspection of map and structure; manual adjustment

### Electron density maps

- Normally:  $2F_o - F_c$  ("the map"),  $F_o - F_c$  (difference density map)
- beware of map bias by the model
- omit ( $2F_o - F_c$ ) maps: try to reduce bias on the map
- kick maps: try to reduce bias on the map