symmetry averaging is carried out on the appropriate submap region, which is then expanded back to a full-cell map prior to each solvent-flattening calculation.

25.2.1.11. *Automated iterative processing*

The most common iterative processes are carried out by shell scripts or command procedures. These procedures merely direct the flow of map, mask, structure-factor and control-data files between the various programs, while controlling the number of iterations in the process. Generally, one does not have to alter these scripts, although expert users may want to in special circumstances.

25.2.1.11.1. *The DOALL procedure*

A script to carry out a standard solvent-flattening run is provided along with a description of the expected input files, output files and examples. Not surprisingly, this *DOALL* procedure does it all. Execution of the script will create a map from an input 'anchor' set of phases, typically obtained by MIR, SIR, or MAD methods, and will then create a solvent mask from the map after zeroing out density near heavy-atom sites. This solvent mask is used in four cycles of solvent flattening, combining the map-inverted phase information with the anchor phases. A new solvent mask is then generated, starting from a map produced with the phases after the first four cycles. Four cycles of solvent flattening using the second solvent mask are then carried out, restarting from the original map and combining with the anchor phases. These phases are then used to compute a new map from which a third solvent mask is built. The third mask is then used for eight cycles of solvent flattening, again restarting with the original map and combining with the anchor phases. Supplied in the script, but commented out, are instructions to carry out an arbitrary number of additional phase extension cycles, and then an arbitrary number of phase and amplitude extension cycles, all using the third solvent mask. The combined phases and distribution coefficients are written to a file after all cycles with a given mask are completed.

25.2.1.11.2. *The EXTNDAVG and EXTNDAVG_MC procedures*

Additional scripts are provided to carry out phase extension and/or NC symmetry averaging iterations. These scripts are executed after completion of a normal solvent-flattening run with the *DOALL* procedure. With the *EXTNDAVG* script, an input number of additional solvent flattening and/or phase combination cycles are carried out, and phase (and possibly amplitude) extension may be requested. Initial and final d spacings are input to the program *SLOEXT* (batch) along with the number of map modification or phase combination iterations per step, where each step represents the extension by one reciprocal-lattice point in each direction if phase extension is to be carried out. The calculations proceed where the *DOALL* script leaves off, starting with a map made from the final phases and using the third solvent mask. If NC symmetry averaging is to be carried out, after each map calculation the appropriate submap is extracted from it and is passed to *MAPAVG* along with the averaging mask. The averaged submap is passed to *BLDCEL*, where it is expanded to a full-cell map, which then is passed to *BNDRY* for solvent flattening. Map inversion and phase combination then proceed normally (although possibly with phase extension). Note that, in general, separate masks are used for solvent flattening and averaging.

The *EXTNDAVG_MC* script carries out the same procedures and options as the *EXTNDAVG* script, except that it is used when carrying out NC symmetry averaging with multiple crystal forms. Starting phase files, anchor phases, solvent masks, averaging masks and control files are provided for each crystal form. For each form, the solvent flattening and phase combination steps are carried out independently with the appropriate data; however, during the averaging step, maps from all crystal forms are involved.

25.2.1.12. *Graphical capabilities*

To facilitate visual evaluation of phasing results and input data, several (mainly interactive) programs are provided within the package. The programs are used to display contoured electron-density or Patterson maps, for interactive editing of solvent or averaging masks, and for visualization of input or difference diffraction data on workstation monitors or terminals. In most instances, hard copies for inclusion in manuscripts are also obtainable. The interactive graphics programs *MAPVIEW*, *PRECESS* and *VIEWPLT* are provided with two versions of each: one for use on Silicon Graphics workstations and the other (indicated by the same program name but ending in _X) for use on any display device supporting the X-Window protocol. The functionality, input and documentation are identical in both versions of each program.

25.2.1.12.1. *Pseudo-precession photographs*

The interactive program *PRECESS* is provided to display diffraction data in the form of pseudo-precession photographs. One can display any zone or step through all zones, with the corresponding intensities mapped to a colour scheme. If a grey scale is selected, the image looks very much like a properly exposed precession photograph taken with Polaroid film. When the cursor is placed near a reciprocal-lattice point, the Miller indices, intensity, standard deviation and d spacing are displayed, allowing one to quickly confirm or identify space groups and Laue symmetry. If a scaled file is input containing isomorphous-replacement or anomalous-scattering data, one can display the corresponding intensity differences instead of the native intensities and quickly visualize the distribution of differences to help assess isomorphism.

25.2.1.12.2. *Interactive contouring or mask editing*

The interactive program *MAPVIEW* can be used to examine contoured electron-density or Patterson maps, as well as to examine, create or edit solvent or averaging masks. Either full-cell *FSFOUR* maps or submaps (including skewed submaps) can be used, although only from the former can any arbitrary region be obtained and reordered interactively. The mask creation and editing functions have been described earlier. The program is very useful for Patterson analysis, evaluation of phasing results and to help decide which region is appropriate for isolating a molecule for use in model building. It is usually crucial for construction of averaging masks, but is also useful for examining or editing other masks.

25.2.1.12.3. *Off-line contouring*

While *MAPVIEW* is extremely useful, there are times when it is desirable to have individual plots available either for comparison, stereo viewing of electron density, or incorporation into documents. The program *CTOUR* (batch) handles these functions and accepts an input *FSFOUR* map or submap. The *CTOUR* program can create any number of plot files in a single run, with each consisting of either an individual section, a mono projection, or a stereo projection, with each projection over different multiple sections. If full-cell *FSFOUR* maps are input, any desired region may be selected, whereas if submaps (including skewed maps) are input, the accessible regions are limited by those present in the input map.

references