

## W0054

**Enhancing the Capabilities of ARP/wARP.** Serge X. Cohen, Krista Joosten, Marouane Ben Jelloul, Victor Lamzin, Anastassis Perrakis, Molecular Carcinogenesis, NKI, Plesmanlaan 121, Amsterdam 1066CX, NL.

As automated protein model building procedures (such as implemented in ARP/wARP, Resolve or MAID) are able to build partial initial models with minimum user intervention, manual interactive building is gradually shifted towards the end of the process. Hence it is a natural trend for automatic building development to spend more effort towards providing a more complete model.

First we propose a new algorithm to estimate the posterior probability of a given amino acid (characterised by its observed topology) to be one of the 20 amino-acid types. These probabilities are then compared to the protein sequences present in the crystal to assign sequence to the present fragments. This Bayesian approach enables us to dock even shorter fragments.

If NCS is present in the crystal, we use docked fragments to derive the NCS operators which are in turn used to perform cross-completion of the different copies. This step has to be done carefully to avoid introducing bias when the NCS is genuinely broken in the structure.

Finally, we propose an algorithm using both electron density and prior knowledge of protein main chain structure to extend main chain fragments at their ends and to build loops between fragments already docked in sequence.

These algorithms are implemented in the new version of ARP/wARP, and enable this version to trace more complete models even at lower diffraction resolution.