Proteins are involved in many essential cellular processes of living organisms. Proteins form macro complexes joining themselves to other proteins to carry out these processes. Therefore, to know the 3D structures of such complexes is of biotechnological interest.

Protein-protein docking algorithms aim to predict how two proteins interact with each other to form a 3D complex. Docking algorithms need to fulfill two main tasks: (1) sampling all the possible relative positions of the two proteins and (2) computing the interaction energy at each position to find the minimum energy (the best solution). Obtaining the interaction energy is a computationally expensive task. We are developing a new algorithm based on the ATTRACT coarse-grained force-field [1] and using a quaternion π-ball representation to accelerate the search of the 3D rotational space.

Based on a preliminary study, we found that a large number of protein interfaces contain at least one pair of atoms at almost their optimal distance according to an empirical force field. Therefore, our idea is to evaluate the difference between a calculated and an experimentally determined 3D structure. Above, we show the rank and RMSD of some of the solutions found by our algorithm.

In order to detect the bead pairs that can lead to steric clashes upon ligand rotation, we compute the differences between the distances. Thus, for all (a, b) in (Receptor, Ligand),

\[
\Delta = d_{ab} - d_{min}
\]

where \(d_{ab}\) is the distance between atoms a and b, \(d_{min}\) is the minimum distance, \(\Delta < 0\) means that the beads will never clash, whereas \(\Delta > 0\) means that the beads might overlap or not (see Fig. 5 and 6).

**Results**

**Conclusions**

The rotational space can be labeled in order to identify unfavorable rotations before computing any energy. Thus, the labeled π-ball can be used as a rotational map avoiding to compute energies at useless rotations. Therefore, the exploration of the rotational space is done in an efficient way. The exploration is exhaustive since the complete rotational space is analyzed and labeled.

**Acknowledgements**

Maria Elisa Ruiz-Echartea is supported by a doctoral bursary (CORDIS) from Inria Nancy Grand Est.

**References**