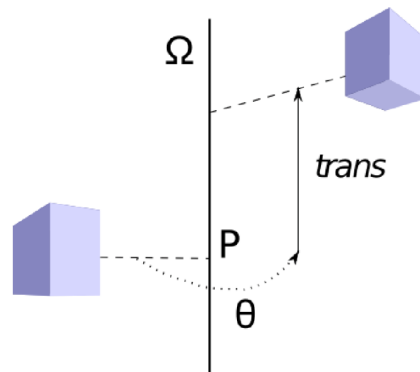


Heligeom: relating interfaces with 3D architectures

Screw organization

A regularly organized oligomer is uniquely defined by the geometry of interaction between neighboring subunits (where the subunit can be a peptide, a protein, a multi-component assembly).

A regular oligomeric assembly necessarily follows a screw organization : it can form either a helix (rotation around an axis coupled to a translation along this axis), a ring or a straight assembly along the axis.



The **helix** is the general case, it is characterized by helical parameters such as the pitch, the number of monomers per turn and the handedness. A cyclic oligomer is a special case of screw assembly, where the pitch is null. The straight assembly is a special case of screw assembly, where the rotation around the axis is null.

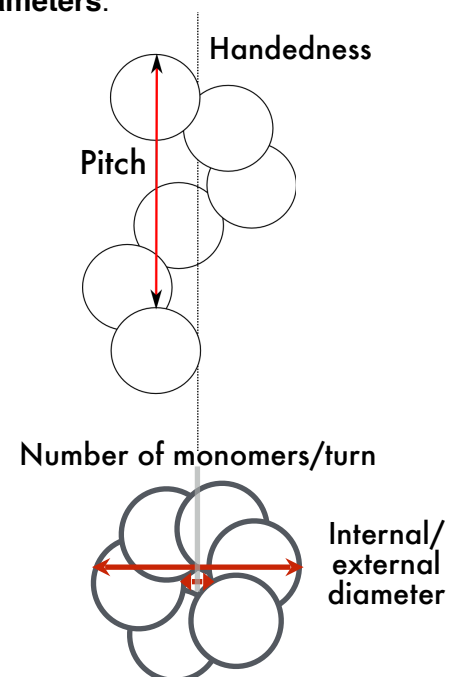
An interface geometry between subunits uniquely defines a 3D organization in terms of pitch and number of monomers per turn. The contrary is not necessarily true.

Helical parameters

A helical assembly is characterized by measurable parameters: the **pitch**, the **number of monomers/turn**, the **handedness**, the internal and external **diameters**.

These parameters can also be derived from the screw parameters.

$$\begin{aligned} nb &= \frac{360}{\theta} \\ pitch &= nb \times trans \\ dir &= \begin{cases} R \text{ if } (\theta \times trans) > 0 \\ L \text{ if } (\theta \times trans) < 0 \end{cases} \end{aligned}$$



Practical session #1 & 2 - from interface to assembly

<http://heligeom.galaxy.ibpc.fr>

This session will be dedicated to the analysis, the construction and the visualization of regular oligomeric assemblies. Training examples are provided on the web server on the form of dimers; alternatively, they can be taken from the PDB <https://www.rcsb.org>

Glutamine synthetase

2GLS_AB.pdb

2gls_EF.pdb

for each file:

Extract the helical parameters starting from two consecutive subunits, either A,B or E,F.

Generate a structure with between 3 and 9 monomers

Compare the parameters obtained in each case.

DmcI - homologous recombination (eukaryotes, meiosis)

Dmc1_AC_R.pdb

Dmc1_AB_H.pdb

for each file:

Extract the helical parameters starting from two consecutive subunits, either A,C or A,B

Generate a structure with 1 turn, 3 turns

Compare the parameters obtained in each case.

RecA - homologous recombination (*E. coli*)

RecA_AB_ATP.pdb

RecA_AB_ADG.pdb

for each file:

Extract the helical parameters starting from two consecutive subunits A,B

Generate a structure with 1 turn, 3 turns

Compare the parameters obtained in each case.

Additional examples taken from the Protein Data Bank

Heligeom Tips & Tricks: the chains and residue ranges can be found on the PDB site <https://www.rcsb.org>

Nipah virus Nucleocapsid: 7NT5

BCL6 transcription factor: 6MXX try chains A,B, A,C and B,D

polymerized form, induced by a small-molecule, that triggers degradation

FtsZ cell constriction, tubulin family: 1W5B

Free exploration...