Ariadna Marín

Project MSI 2 – Water chemical potential

Code explanation:

In order to create a volumetric file which contains information on the position of water molecules, I performed the following steps:

1) Locate all the subfolders within the current directory and store them in a list.

2) Create a for loop that iterates through all these folders and, if a “structure.pdb” file is present, computes the occupancy matrix.

3) In order to compute this matrix, I aligned each PDB file + trajectories with a reference molecule (“2x16” centered at the origin). Afterwards, I used wrap to confine all water molecules into a cube.

4) Extract the coordinates of oxigens from H_2O and set to zero some abnormal points located very far from the molecule using a mask. The effect of this operation does not alter the results, because the number of points moved is really small.

5) Iterate over each atom (i) of each trajectory (t) to get its (x,y,z) coordinates and store them into a 3D matrix. The counts are afterwards converted into probabilities. It is important to note that a translation has been applied to the coordinates to avoid negative indexes.

6) The probabilities obtained for each folder with a structure are averaged and Gibbs free is calculated.

7) Two different .cube files are generated: one for the normal data and another one that has been smoothed using a Gaussian filter (before Gibbs calculation). Minimum and maximum coordinates of the cube are computed to undo the translation that has been previously applied.

IMPORTANT:

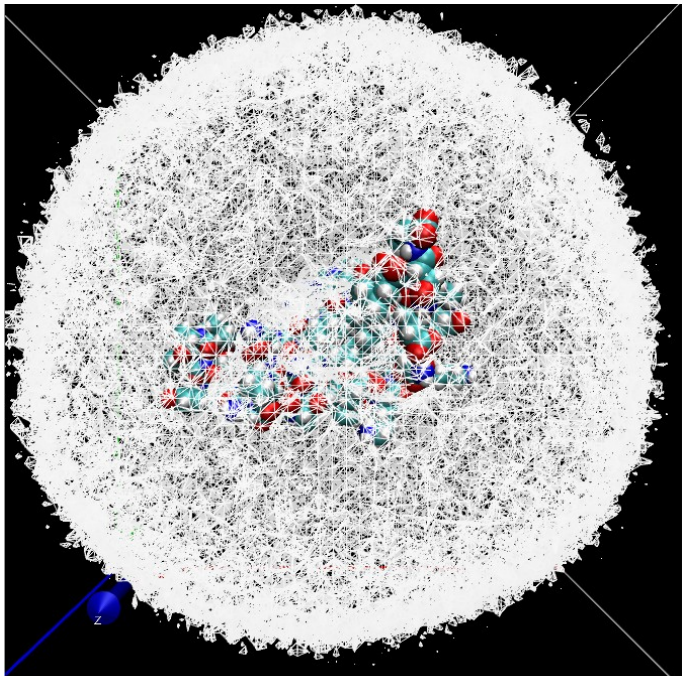
To run the code, the subfolders with the PDB structures need to be placed in the folder where the code is. Otherwise, the following lines have to be modified:

```
path = [name for name in os.listdir(".") if os.path.isdir(name)]
mol_ref = Molecule('./2x16/structure.pdb')
```

Ariadna Marín

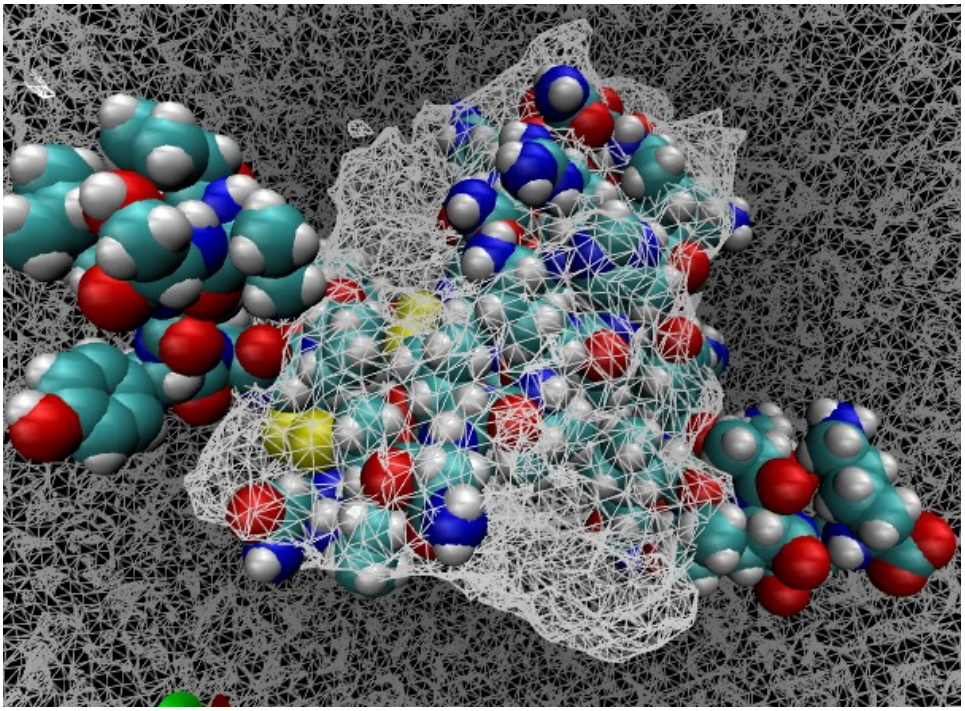
Results:

Normal mesh for 2x16



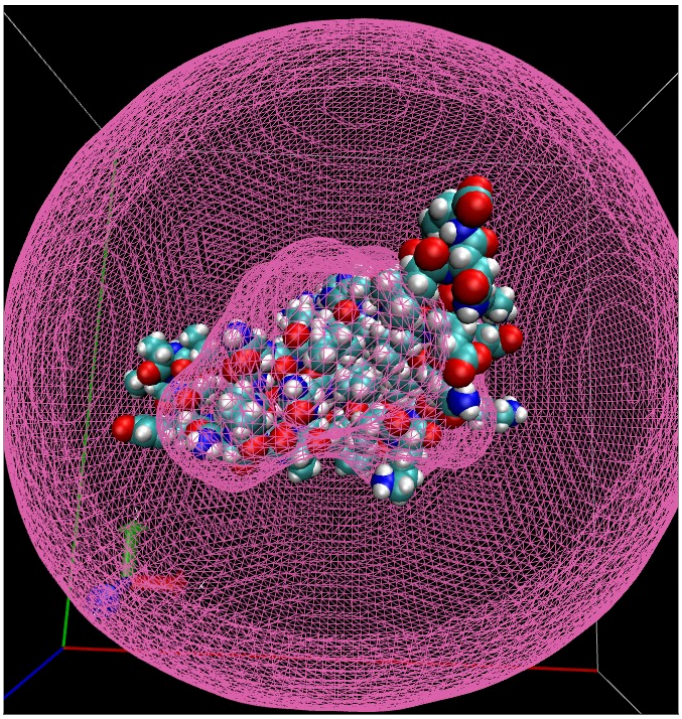
Exterior view of the volume with water.

Area with maximal water density is located around the central part of the protein, leaving out the lateral chains (which are more mobile and change their position through the trajectory).



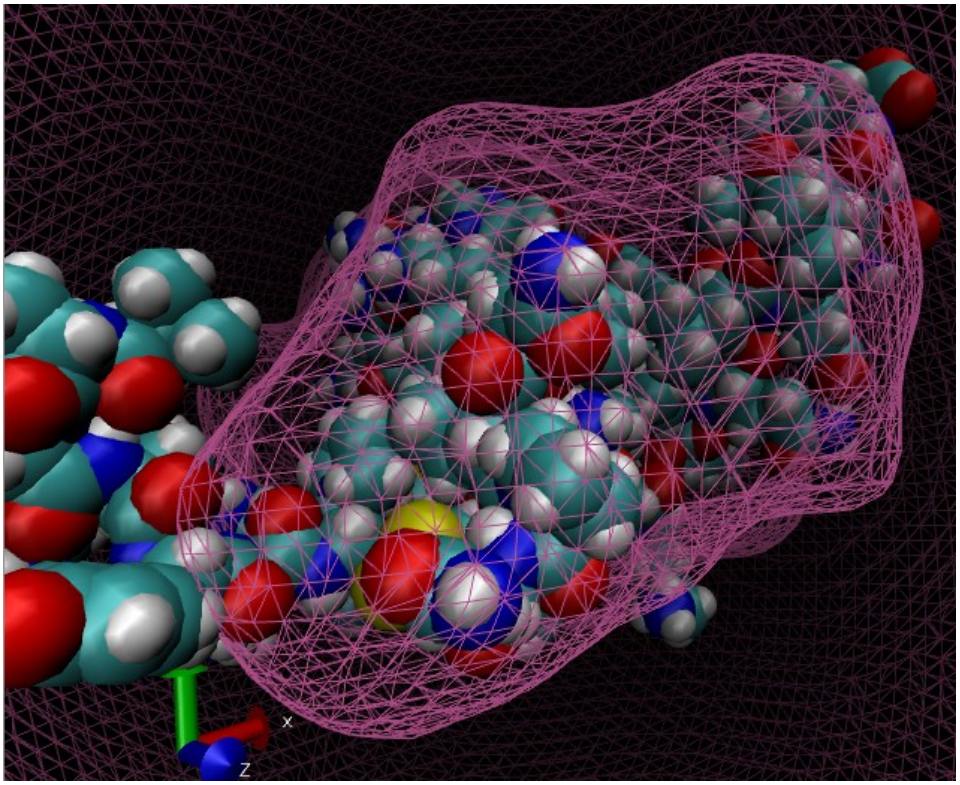
Ariadna Marín

Filtered mesh for 2x16



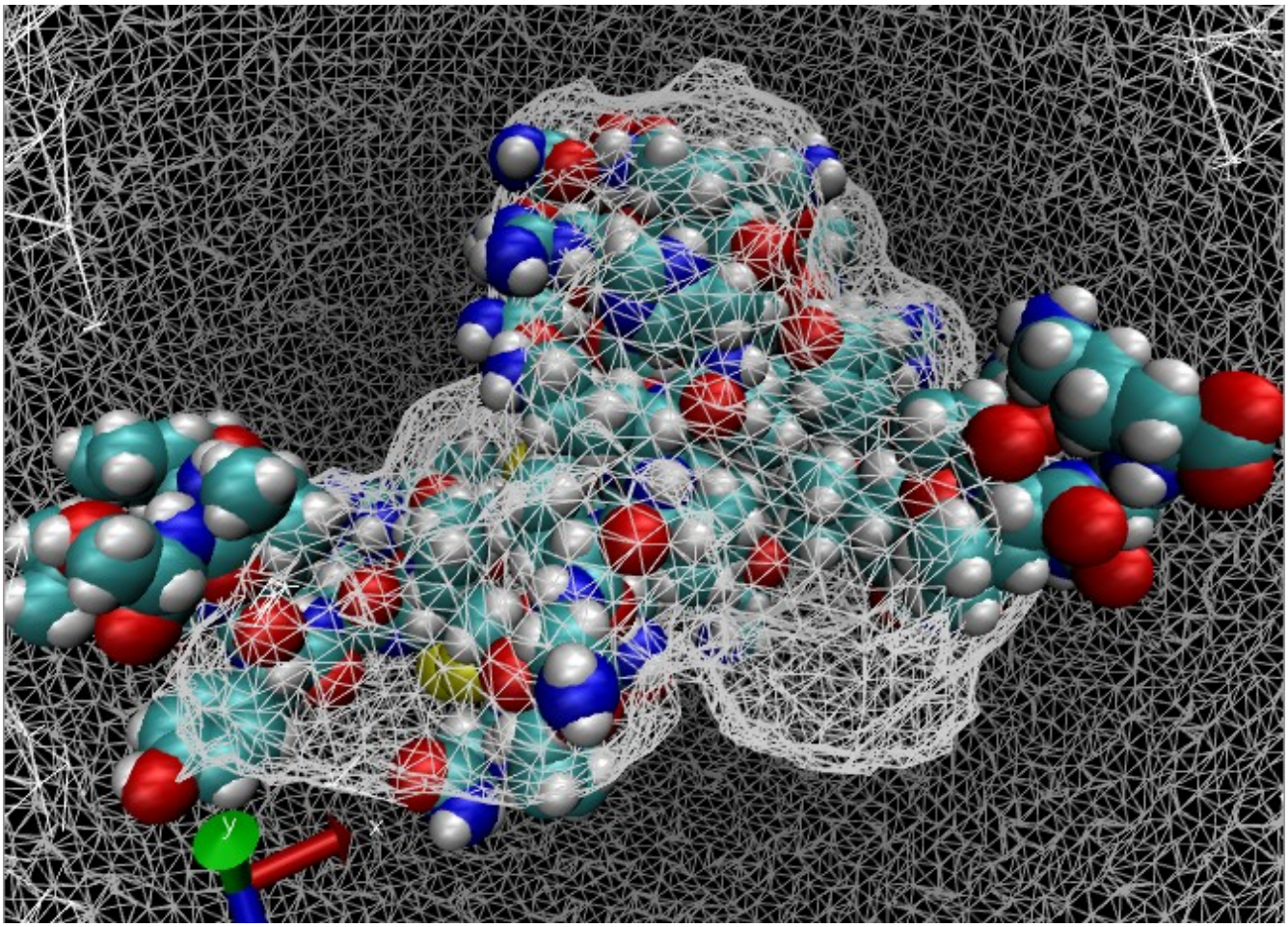
The surface becomes much smoother after the application of the Gaussian filter.

The volume with high water density has also become smoother.



Ariadna Marín

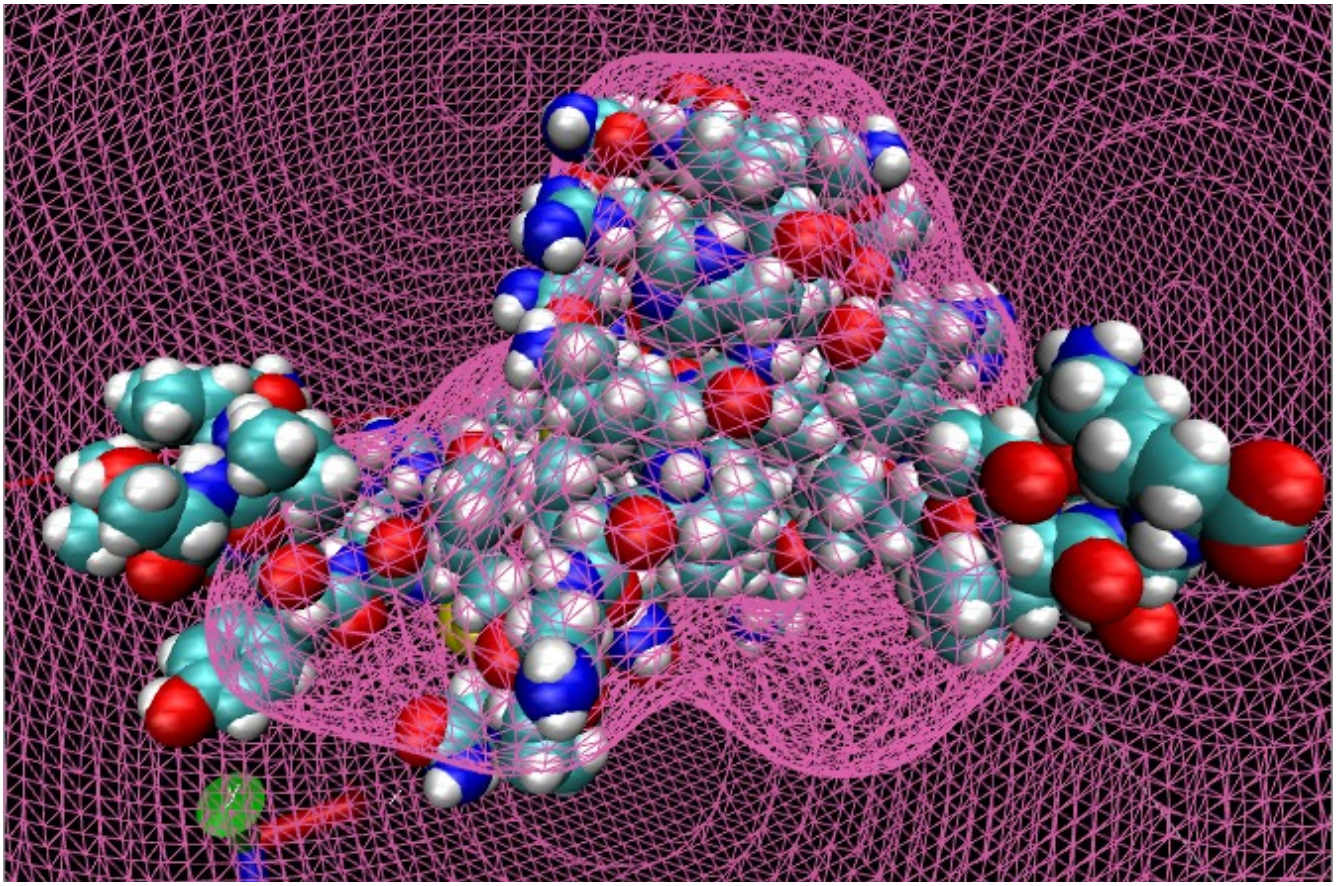
Normal averaged mesh



By imaging the final mesh with an isovalue of 7.5, we can see that the volume with high density has increased, covering a bit more the lateral chain of the protein.

Ariadna Marín

Filtered averaged mesh



By filtering the values we get, once again, a much smoother mesh.