## 1.1 APL@Voro Workflow

Figure 1 - 4 show the workflow and the internal logic of APL@Voro in certain program steps. In Figure 1, the general workflow of APL@Voro is shown. Figure 2 shows the logic during the project creation, Figure 3 presents the procedures performed while parsing user supplied files and data and Figure 4 shows a flowchart of the procedure performed to insert single atoms into an initial triangulation.

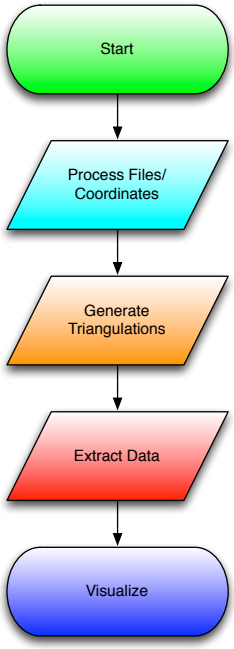



Figure 1: Workflow of APL@Voro. Rounded symbols mark program states with user dialogs. Parallelograms mark the program states, where calculation is carried out. The colors refer to the respective Figures Fig. Supporting Information 2 (green), Fig. 3/4 Supporting Information (cyan), Fig. 5 (orange) and Fig. 6 (red). The "Visualizing" (blue) step is described together with the APL@Voro's user interface in section 3.4 *User Interfaces and Visualizing Data*.

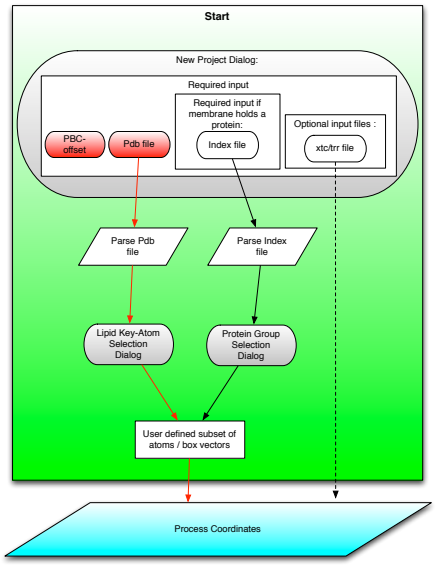



Figure 2: Flowchart of the internal logic of APL@Voro during the project creation. Grey rounded symbols mark program states with user dialogs. Parallelograms mark the program states, where calculation is carried out. The miminum input configuration is marked in red (PBC-offset, Pdb file). The resulting minimum workflow is marked with red arrows.

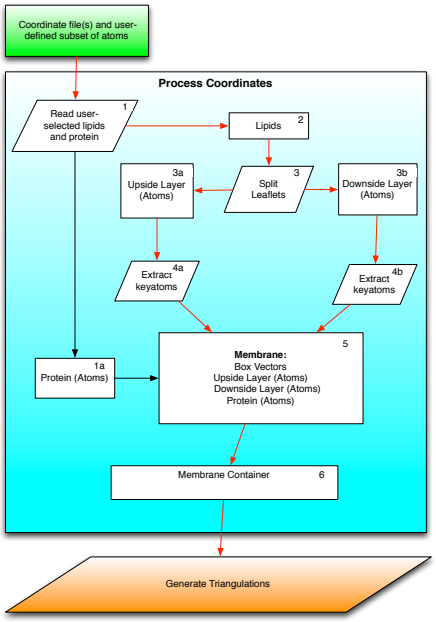



Figure 3: Flowchart of the internal logic of APL@Voro in the program state where coordinate files (PDB, XTC/TRR) are processed. Rectangles mark internally stored data structures. Parallelograms mark program states, where calculation is carried out. Red arrows mark the programs flow for a minimal configuration (i.e. without protein).

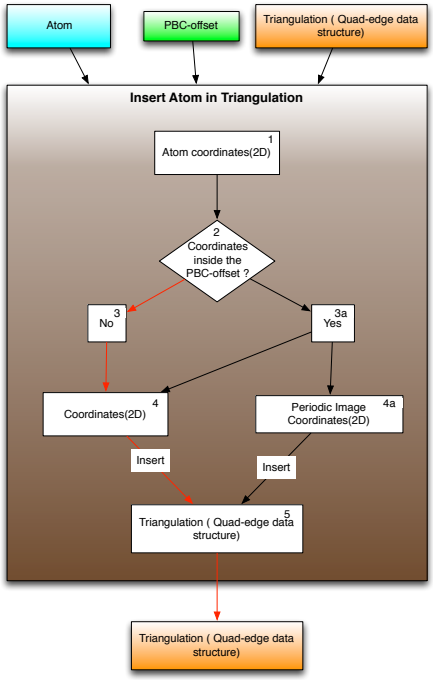



Figure 4: Flowchart of the internal logic of APL@Voro for the "Insert Atom in Triangulation" procedure. Rectangles mark internally stored data structures. Parallelograms mark program states, where calculation is carried out. Rhomboids mark decision states of the program. Red arrows mark the programs flow for a minimal configuration (no periodic image is created). The "Insert Atom in Triangulation" procedure is a sub-procedure of the calculation of the triangulations.

## 2 APL@Voro Screenshots

Figure 5 - 7 show the GUI of APL@Voro. The dialogs presented in figure 4 and 5 are presented to the user during the setup process of a new project. Figure 6 shows the dialog to create a selection criterion. The plotting window for three-dimensional plots is shown in Figure 7.

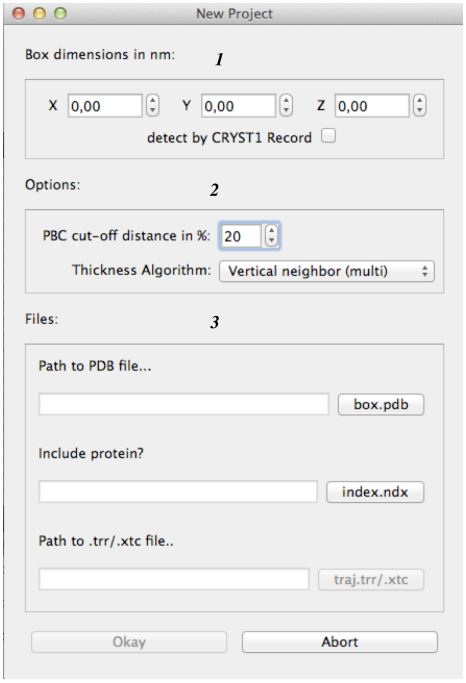
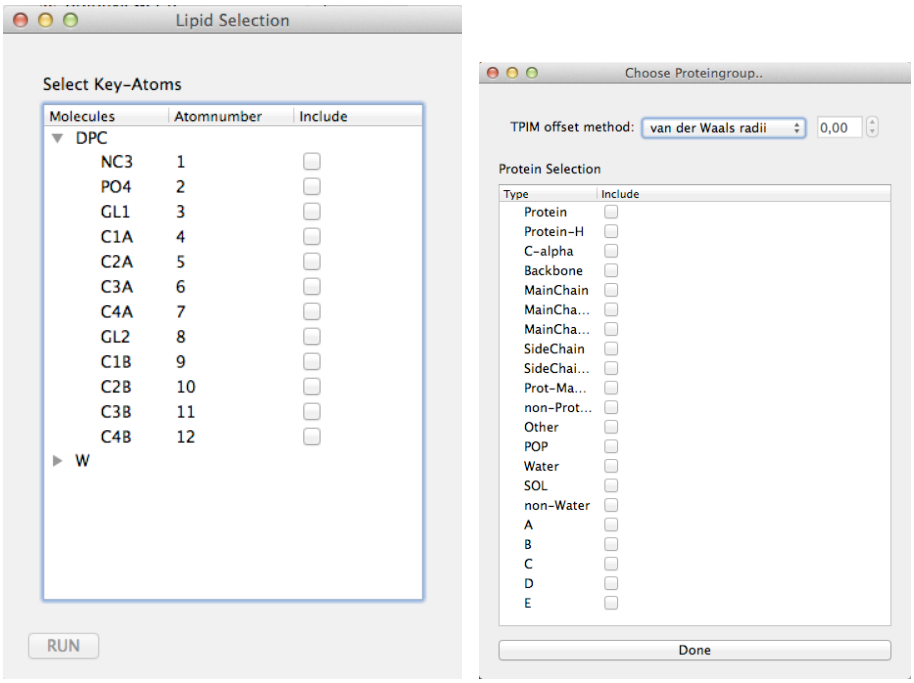



Figure 5: Screenshot of the "New Project" dialog. The dialog is used to enter the coordinate files and the index file. Box dimensions can be entered by the user or detected by the CRYST1 Record of the respective PDB file. Additionally, the user can change how to treat periodic boundaries and choose the algorithm for the calculation of the membrane thickness.




(a) Dialog for lipid key-atom selection.

(b) Dialog for protein group selection

Figure 6: Screenshots of the user dialogs to select lipid key atoms (a) and protein groups (b). In Figure (a), the atoms of a DPPC molecule modeled with the MARTINI force field are displayed. Key-atoms can be selected by clicking the respective checkbox to the right of an entry. In Figure (b), the contents of a Gromacs index file are listed. The user can select one or multiple groups that are handled by APL@Voro as a single protein. At the top of Figure (b), the user can change the TPIM offset method and thus, modify the height of the triangular prism used in the TPIM procedure.

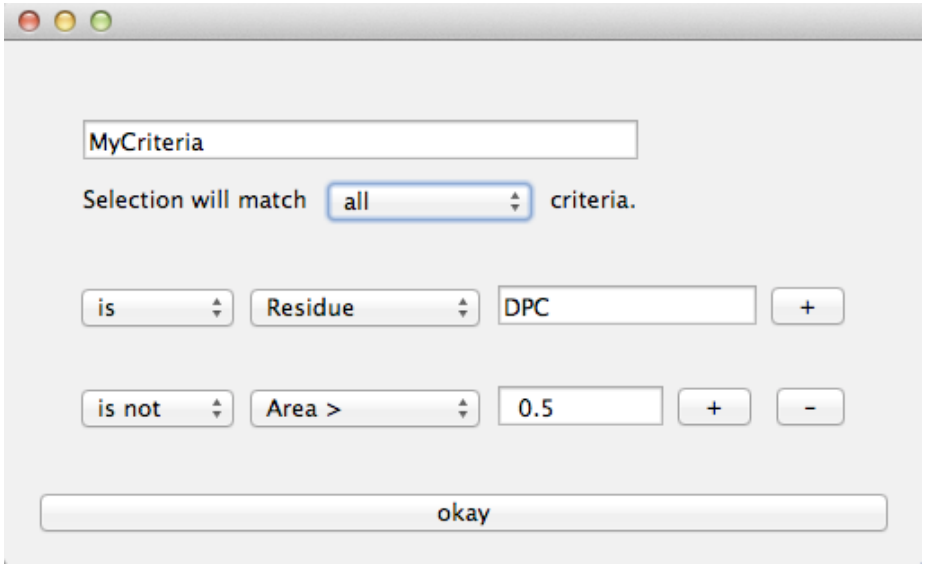



Figure 7: Screenshot of APL@Voro's dialog to define a selection model. The defined selection model will be named "MyCriteria" and will automatically select all Voronoi cells referring to DPC lipid with a calculated area which is lower than 0.5 $nm^2$.

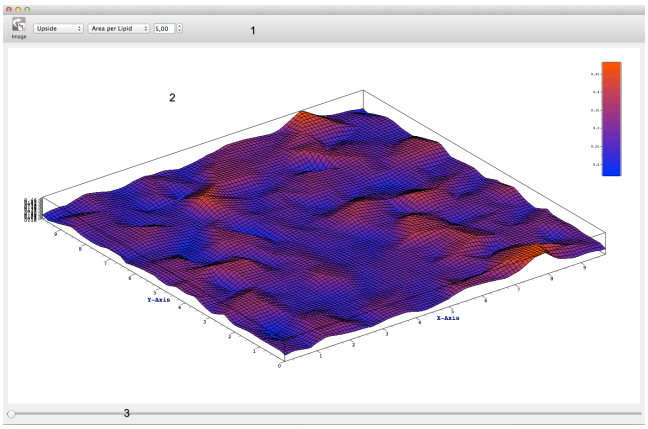



Figure 8: Screenshot of APL@Voro's plotting window for three dimensional plots. Different plots can be selected and scaled in the movable menu bar (1). Every plot is displayed together with a legend in the plotting area (2). The resolution of the grid can be changed using the control slider at the bottom of the window (3).

# 3 XML file export

The .xml files exported from APL@Voro follow the XML Schema shown in Listing 1. The root element of the .xml file is the "$< LAYER/ >$" element. It holds an attribute "Time" with a floating value referring to the time in $ps$. The root element holds several "$< Atom/ >$" elements referring to the atoms used to construct the triangulation. Every atom holds one attribute for the atom number ("Number"), one for the atom name ("Atomname"), one for the residue name ("Resname") and one for the residue number ("ResNumber"). The "$< Atom/ >$" element itself contains five elements: "$< X/ >$", "$< Y/ >$" and "$< Z/ >$" for the respective coordinate in $nm$, "$< Area/ >$" and "$< Thick/ >$" for the calculated area (in $nm^2$) and the calculated thickness at this point (in $nm$).

Listing 1: XML-Schema for the XML files exported by APL@Voro

```
<?xml version="1.0" encoding="utf-8"?>
<xs:schema attributeFormDefault="unqualified" elementFormDefault="
    qualified"
   xmlns:xs="http://www.w3.org/2001/XMLSchema">
  <xs:element name="points">
    <xs:complexType>
      <xs:sequence>
        <xs:element maxOccurs="unbounded" name="point">
          <xs:complexType>
            <xs:attribute name="x" type="xs:unsignedShort" use="
                required" />
            <xs:attribute name="y" type="xs:unsignedShort" use="
                required" />
          </xs:complexType>
        </xs:element>
      </xs:sequence>
    </xs:complexType>
  </xs:element>
</xs:schema>
```