PyLasso workshop June 24, 2021

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Short introduction

PyLasso website: https://pylasso.cent.uw.edu.pl. According to the page:

"The PyLasso detects all types of lassos based on techniques developed in (link), which involve analysis of surfaces of minimal area spanned on closed loops, and the number and directions of segments piercing such surfaces. The plugin enables to detect different types of covalently closed loops. A user can also define news loops, either by selecting a part of the backbone forming a loop, or typing sequential numbers of two atoms that form a bridge. Detected lasso configurations, including the minimal surface and piercings, are represented graphically in the PyMOL environment. The plugin is equipped with additional tools that facilitate analysis of lassos, in particular structure smoothing (which simplifies the structure by ignoring e.g. helices and sharp turns) and minimal surface smoothing."
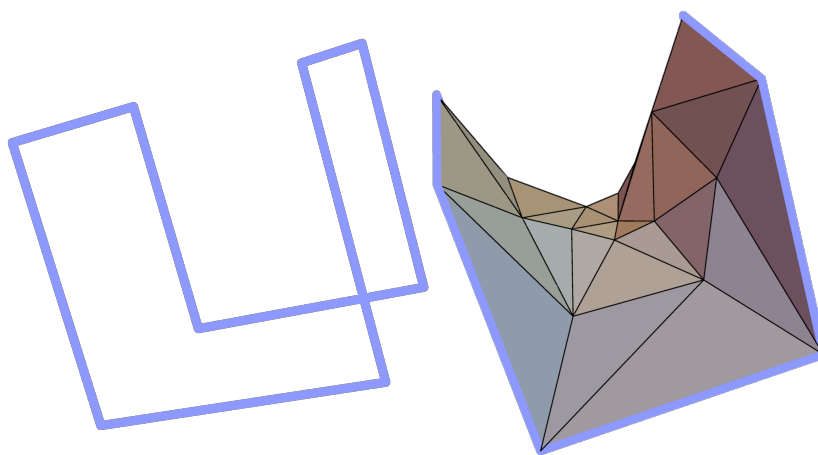
Figure 1. Exemplary frame without (on left) and with minimal surface spanned on it.
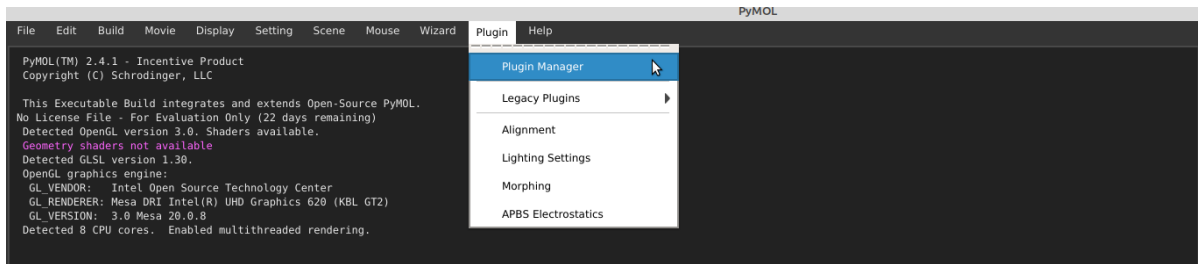
Installation

PyLasso is PyMOL plugin, therefore requires PyMOL ☺. Please download correct plugin version depending on your system version and Python version:
For Python >2.7: Package for linux, Package for Mac OS X, Package for Windows.
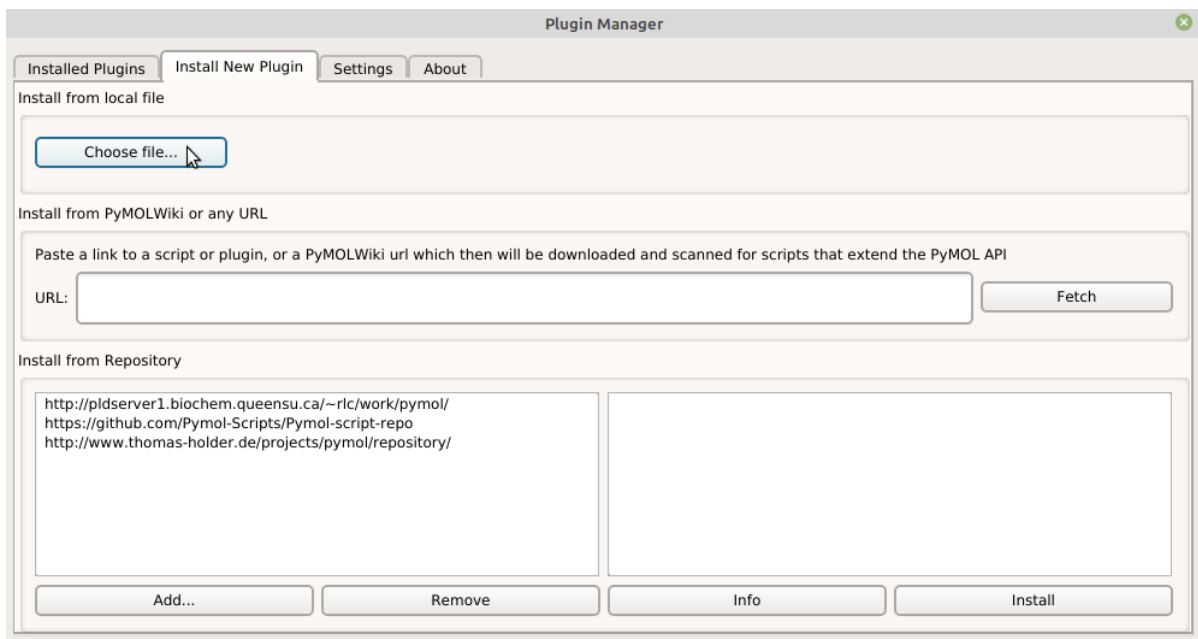
For Python 2.7: Package for linux, Package for Mac OS X, Package for Windows.
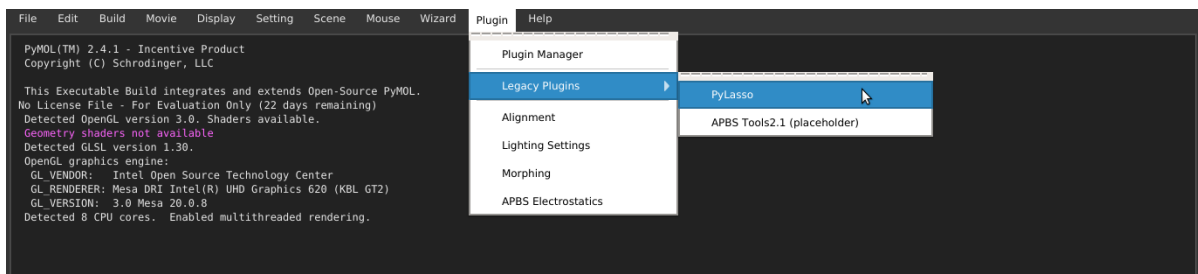
 1. Unpack your package;

2. run PyMol

3. run plugin Manager

4. Go to install new plugin and choose file `__init__.py` for unpacked folder
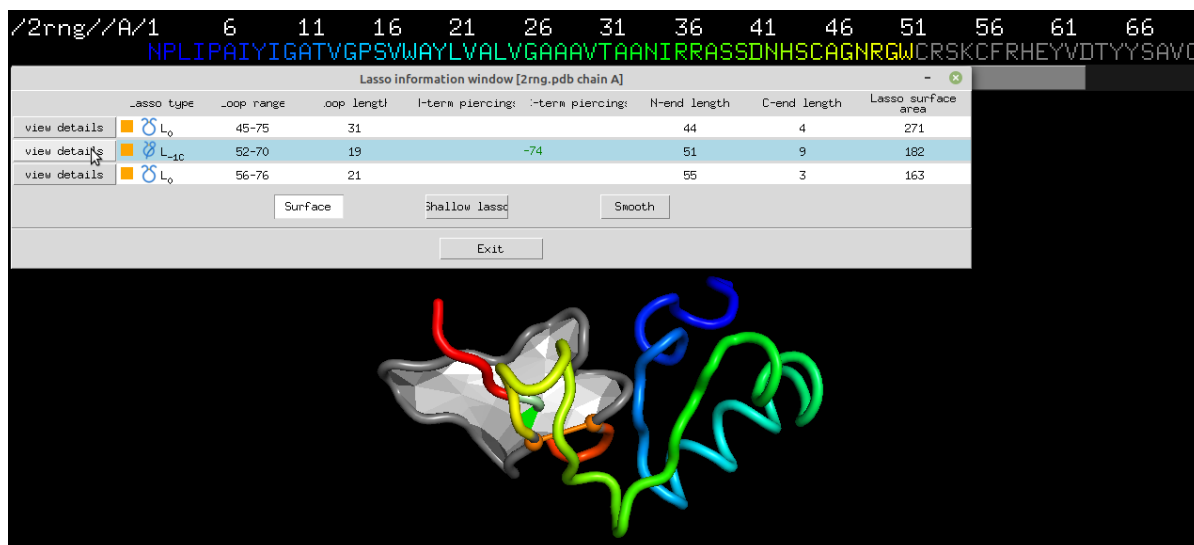

5. Finally run PyLasso and load chosen pdb file. If the file consists of many structures you will be asked if plugin should load files as a trajectory.
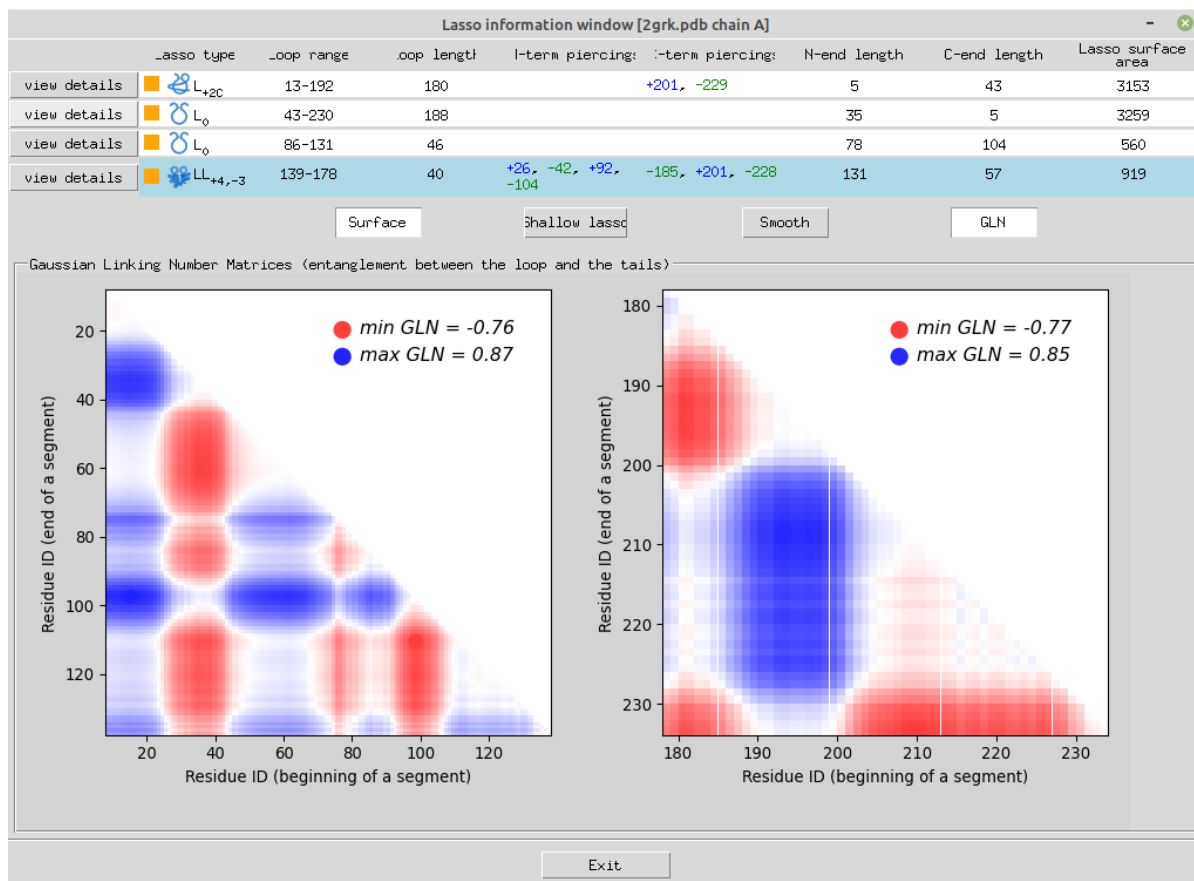
Usage

1. Load lasso peptide Astexin `2rng.pdb` and press "Proceed". Then choose the lasso you want to see.

2. PyLasso can calculate GLN matrix. Exit PyLasso and run it again loading `2grk.pdb`. Mark "Calculate GLN". Then choose one of the loops and press "GLN". Wait patiently until the matrix show up, because any unnecessary operations may crash PyMol during calculations.

3. Lets check other options during loading the structure. Load `2rng.pdb` (or other pdb structure). Most importantly you can change rules in which lassos are found. Defaultly the lasso is classified as shallow if crossing is sequentially too close to:

   - another crossing;
   - its lasso loop;
   - its tail end.

   These distances can be changed (e.g. to 0, for classifying all lassos as not shallow) after unmarking "Stable lasso" option.

4. You can also create your own loops by connecting two residues. It can be done by changing a "Method to set a loop closing": choose two atoms to form a bridge. You can load these residues by:

   - writing their indices;
   - marking them in structure view in PyMol panel;
   - marking them in sequence view in PyMol panel.

   Either way unmarking "Ignore an inappropriate length of bridge in Ca-Ca bond" may be advised.