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."

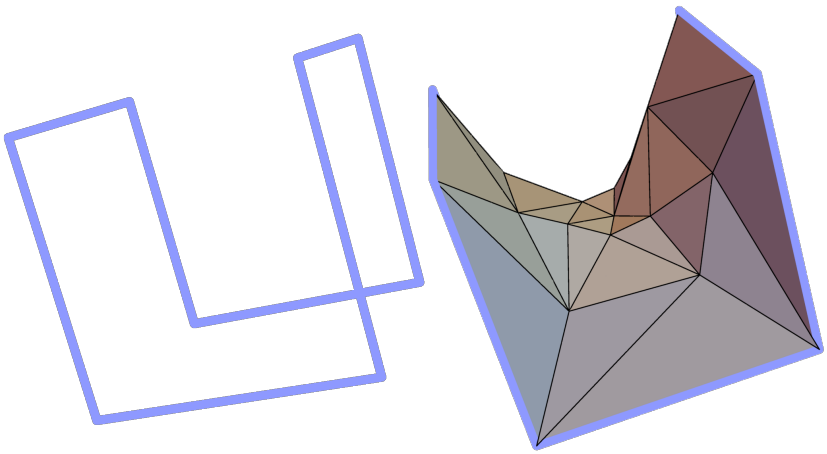

Figure 1. Exemplary frame without (on left) and with minimal surface spanned on it.

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.

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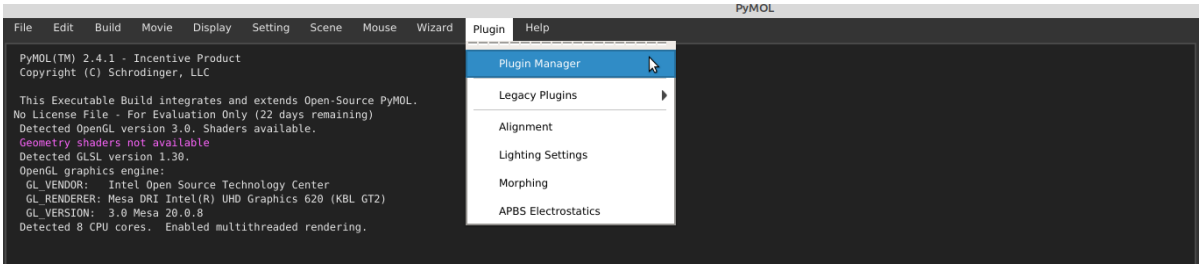
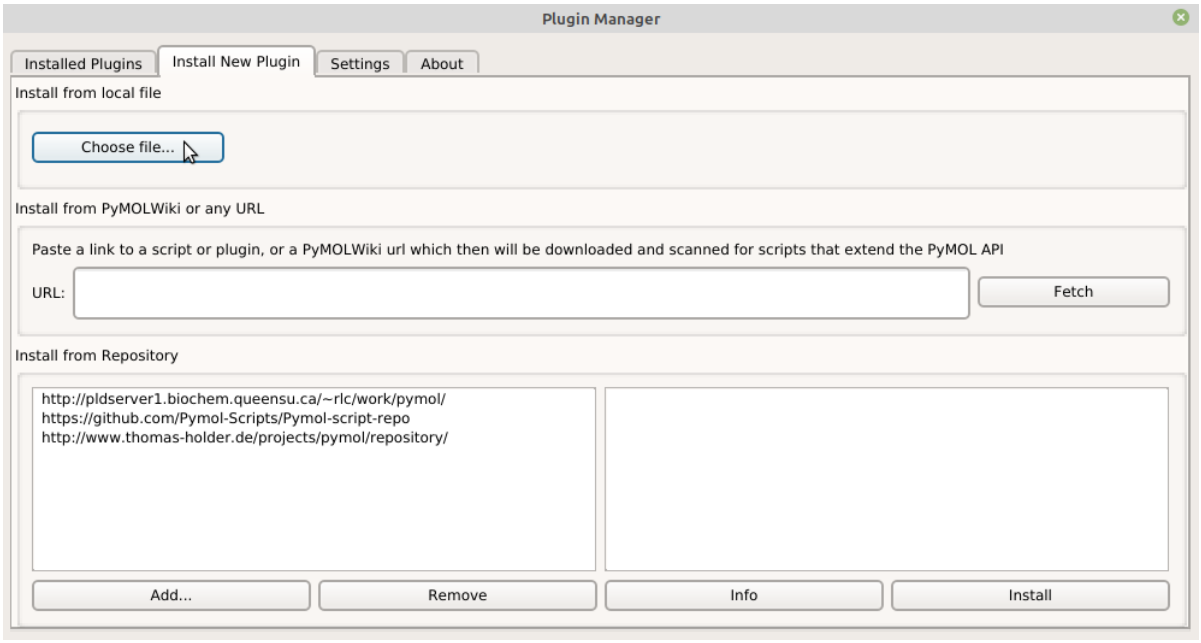
1. Unpack your package;

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