Polymer-Elasticity v2.2.0

# General Information

The polymer-elasticity script can be used to fit the model of the extended, freely jointed chain to results of force-clamp experiments (and only this functionality has been designed for this script). The model is as follows [1, 2]:

Where represent the force-dependent expansion of the measured molecule and represent the force applied in z-direction to the molecule. The free parameters of the model are

* : Segment-Elasticity in
* : Contour-Length in
* : Kuhn-Length (Monomer-Length) in

The constant Parameters are the Boltzmann constant as well as the absolute Temperature .

This model is fitted to the plotted inverse function (path vs. force) at the data range selected in *polymer\_elasticity*.

# Changelog

* The Help is now located under the Menu Point “Polymer Elasticity” as a Browser Version

# System requirements

## Necessary Programs

* Matlab (= 2019a)
* Python (= 3.7)

## Necessary Matlab Apps

* Kraftkurven.mlapp

## Necessary Matlab Scripts

* Polymer\_elasticity (>= 2)

## Necessary Librarys

* Utility Function Library

# User Guide

## Start of the Program

To start the script *polymer\_elasticity*, there are two ways:

* Type “polmer\_elasticity” in the MATLAB-Command window
* Open the Script *polymer\_elasticity* in the MATLAB-Editor and Hit “Run” or press “F5”

What follows is the opening of a Figure called “Polymer Elasticity and the creation of an empty Axes together with several Gui-Elements (for more Details about the Gui-Elements, see the Section Miscellaneous)

## Load Force-Curves from Text-files

To import Force-Curves from Text-files, the MATLAB-App *Kraftkurven* gets utilized. To open this App, go to the menu point "Polymer Elasticity" in the Figures menu band and Click on "open Kraftkurven". Next, hit the "Load"-Button und choose a folder where appropriate Text-files are located. Make sure, that the Text-files meet the following points:

* The Text-files are Exported from the "JPK Data Processing"-Software (version 5 or later) from Bruker (formally known as JPK Instruments AG)
* Export the Text-files with full header settings

For Force-Clamp-Experiments it might be advantageous to choose the option "retrace" in the "Curve Segments to Plot"-Dropdown menu. This option shows only the part with the Clamp-Event of the exported Force-Curves. To use the *freely jointed chain* Model, the default Values in the Dropdown menus for x- and y-channels should remain untouched.

## Create the Variable DataSelection

If the Force-Curves loaded properly, MATLABs Plot tools together with a Figure, showing all Force-Curves located in the chosen folder, would open. In Order to create „DataSelection“, follow the next Steps:

1. Right-click on **any** of the staggered Graphs and choose "Graphen Staffeln" (in the "Offset"-Dialog just hit "Ok")
2. Right-click on a **certain** Graph, which should be evaluated and hit the menu point "Öffne Graph in neuer Abbildung"
3. In the new Figure disable all Figure Tools
4. Right-click on the white space around the Graph
5. Choose a specific Selection Type and mark the Region on the Graph which is related to the Extension of a Polymer
6. Right-click on the selected Data Range and hit "To Workspace" to create *DataSelection* in MATLABs base Workspace

In the Base-Workspace of MATLAB the following Variables should now exist:

* **Data**
  + Structure with Program specific Data created from *polymer\_elasticity*
* **Gui\_Elements**
  + Structure with Gui\_Elements created from *polymer\_elasticity*
* **ForceCurves**
  + Stucture with all loaded Force-Curves from *Kraftkurven*
* **DataSelection**
  + nx2 MATLAB-Vector describing the Region of Interest of a Force-Curve, created via *Kraftkurven*

## Fit the Model to the loaded Data

1. Hit the Button "Reimport DataSelection" to show *DataSelection* *polymer\_elasticity*
2. Choose an appropriate Starting Point for the Clamp-Event either by Left-clicking on a point on the Graph or by entering a Value in the xoffset/ yoffset cells in the table (where it sys "NaN" at the beginning)
3. Chose an appropriate Fit Range for the Model. This can be done either by hitting the Button "New Fit Range" and dragging an Region of Interest or by entering Values for the Cells "Xl" and "Xr" (Where it says "NaN" at the beginning)
4. If the Fit doesn´t start automatically, hit the Button "DoFit" on the Slide-Panel (">>"-Button)

## Adjusting the Fit parameters

If the Default-Values for the fit were inappropriate, the Parameters for the Fit would be adapted in the slide-panel. The Slide-Panel is at the beginning hidden behind the Button ">>". Initial Values for the Fit can be adjusted by entering new Start Values for variable and constant Parameter directly to the "Value"-Columns of the Variable- and Constant-Parameter Tables. Additionally, variable Parameter can be fixed at a certain Value by checking the Box "hold" for the corresponding Parameter. This specific Parameter remains untouched during the Fit. By default, the variable Parameters and are fixed at the initial Values, remains free (constant Parameters are fixed per definition and can´t be changed to variable ones). If Values were entered to the tables (this is valid for all tables), the Fit must be reevaluated by pressing the "DoFit"-Button.

# Miscellaneous

## Load new Data

If the Data in the Variable *DataSelection* changes, it´s necessary to reimport the Data to *polymer\_elasticity* by pressing the Button called "Reimport DataSelection". Thereafter the new Graph will appear in the Figure. All Offsets, Fit ranges and Fit representations will be deleted.

## Delete the Fit range

To delete the actual Fit Range, press the Button "Delete Fit range". This will only delete the Fit Range and the Fit Representation. All Offsets remain unchanged.

## Save Figure Elements

To get a "good looking" Version of the Elements in the Figure, right-click on the white Background of the Figure. in the Context Menu choose "Save Figure" and MATLABs Plot Tools will open.

# Terminology

* **Ks Fit**
  + Means the fitted Segment Elasticity of the investigated Molecule
* **Lc Fit**
  + Means the fitted Contour Length of the investigated Molecule
* **lk Fit**
  + Means the fitted Kuhn Length of the investigated Molecule
* **Clamp Length**
  + "Lc Fit" + x-Offset; means the Position of the Clamp-Event in the Coordinate System
* **Xl**
  + Left Border of the Fit Range in %
* **Xr**
  + Right Border of the Fit Range in %
* **Distance**
  + Distance between Xl and Xr in %

References

[1] A. Janshoff, M. Neitzert, Y. Oberdörfer, and H. Fuchs, “Kraftspektroskopie an molekularen Systemen: Einzelmolekülspektroskopie an Polymeren und Biomolekülen,” *Angewandte Chemie (International ed. in English)*, no. 112, pp. 3346–3374, 2000.

[2] M. I. Giannotti and G. J. Vancso, “Interrogation of single synthetic polymer chains and polysaccharides by AFM-based force spectroscopy,” (eng), *Chemphyschem : a European journal of chemical physics and physical chemistry*, vol. 8, no. 16, pp. 2290–2307, 2007.