Center for Energy Resources
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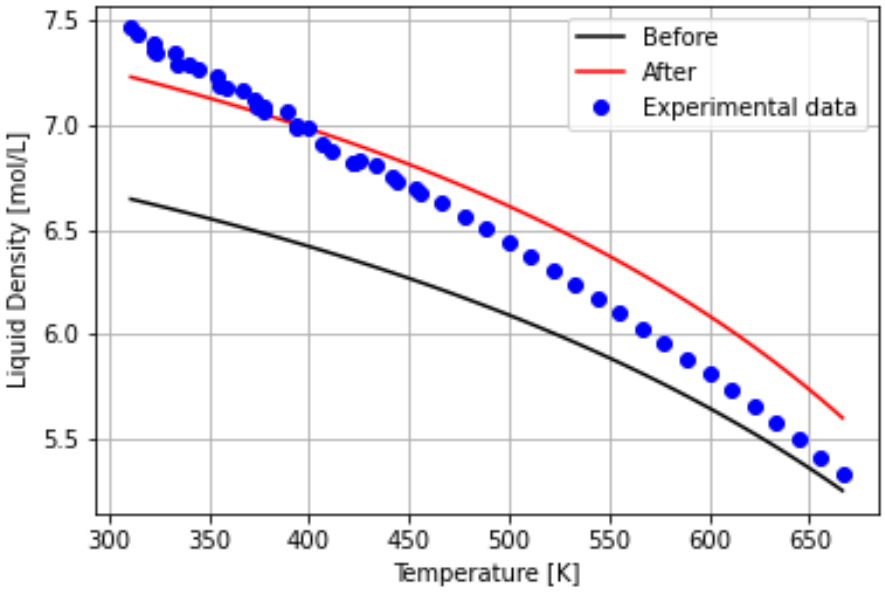
PyTherm

Thermodynamic Phase Equilibria Modelling in Python

User Guide, Edition 1



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Thermodynamic Phase Equilibria Modelling in Python

User Guide, Edition 1
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[John Towne], [unknown title], [Collaborator from USA]
Contributed with optimization functions, and so on...

Contents

1 Introduction to PyTherm

2 Installation of Python and Packages

2.1 Installing Python

2.1.1 Python

Using PyTherm requires Python version 3.8.3 or higher. The newest releases of Python may be found on the official website: https://www.python.org/. However, we recommend installing Python by installing Anaconda, which include the latest version of Python in its installation.

2.1.2 Anaconda

It is strongly adviced to use Anaconda when using PyTherm . https://www.anaconda.com/products/individual

2.2 Installing IDE (Integrated Development Environment)

2.3 Installing relevant packages

2.3.1 lmfit

A python package used in parameter optimization is *lmfit*, which may be installed by using the following guide

1. Open Anaconda Prompt
2. Type `pip install lmfit` in the window
3. Press enter, and let the installation commence.
4. If any error occurs, consult the following link for in-depth installation guide: https://lmfit.github.io/lmfit-py/installation.html

The use of this package also requires the installation of *NumPy*, *SciPy*, *asteval* and *uncertainties*, however these are installed automatically if `pip install lmfit` was used.

3 Jupyter Notebook

3.1 How to open Jupyter Notebook

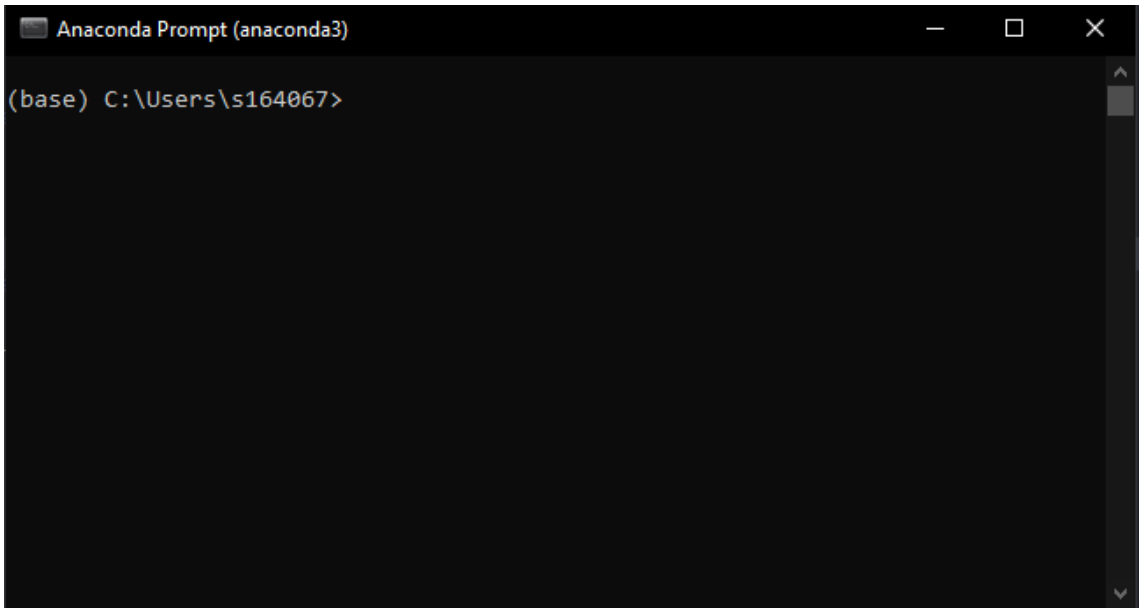


Figure 3.1: Caption

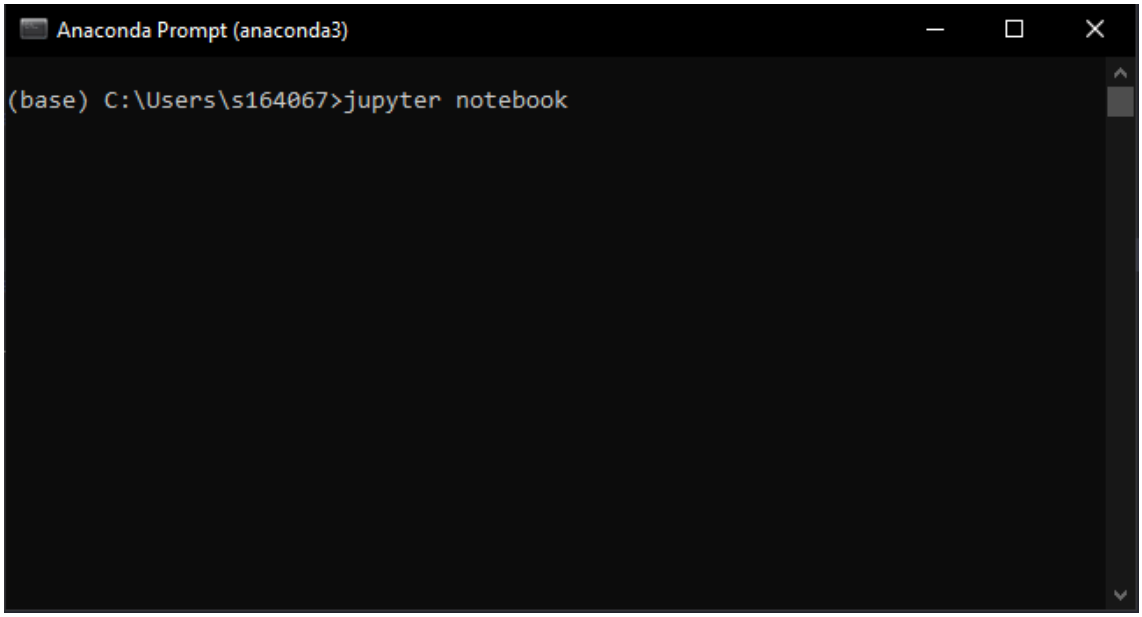


Figure 3.2: Caption

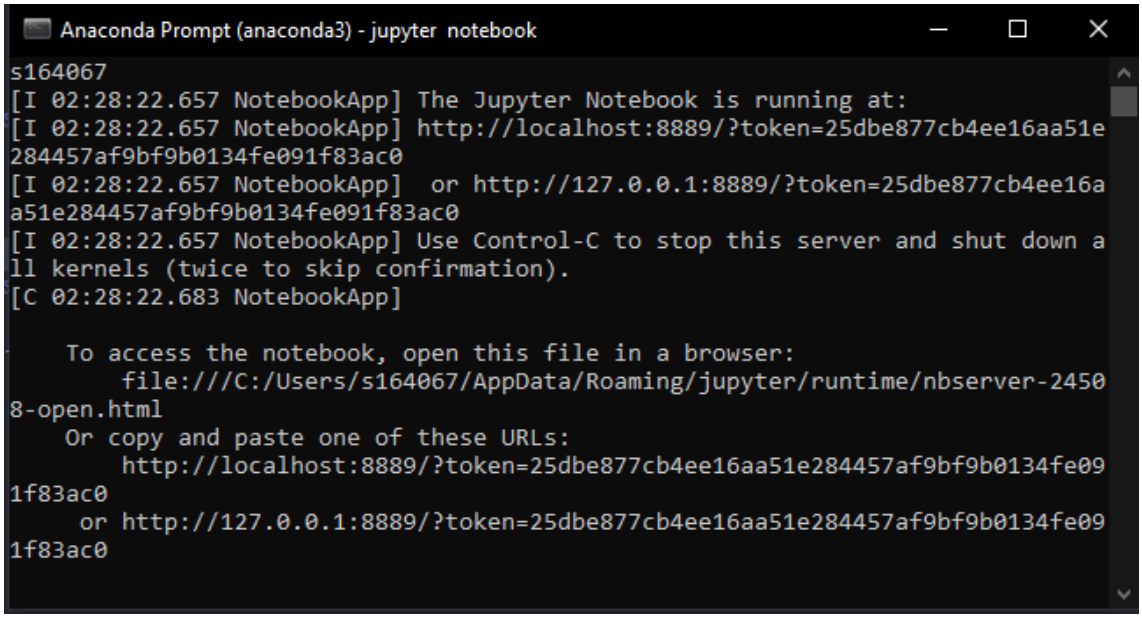


Figure 3.3: Caption

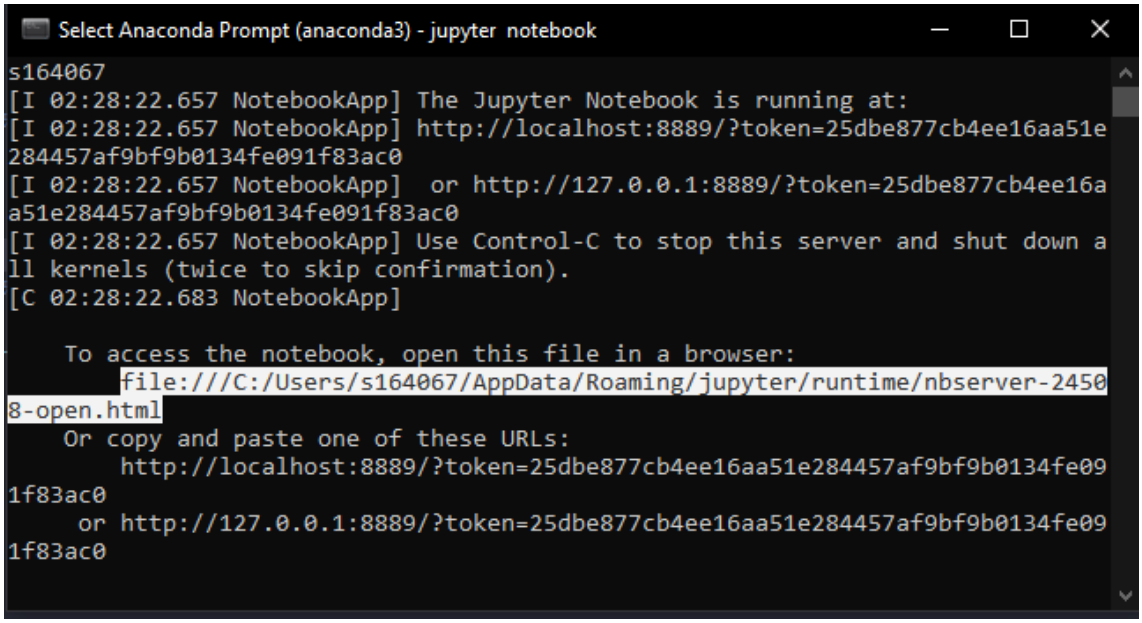


Figure 3.4: Caption

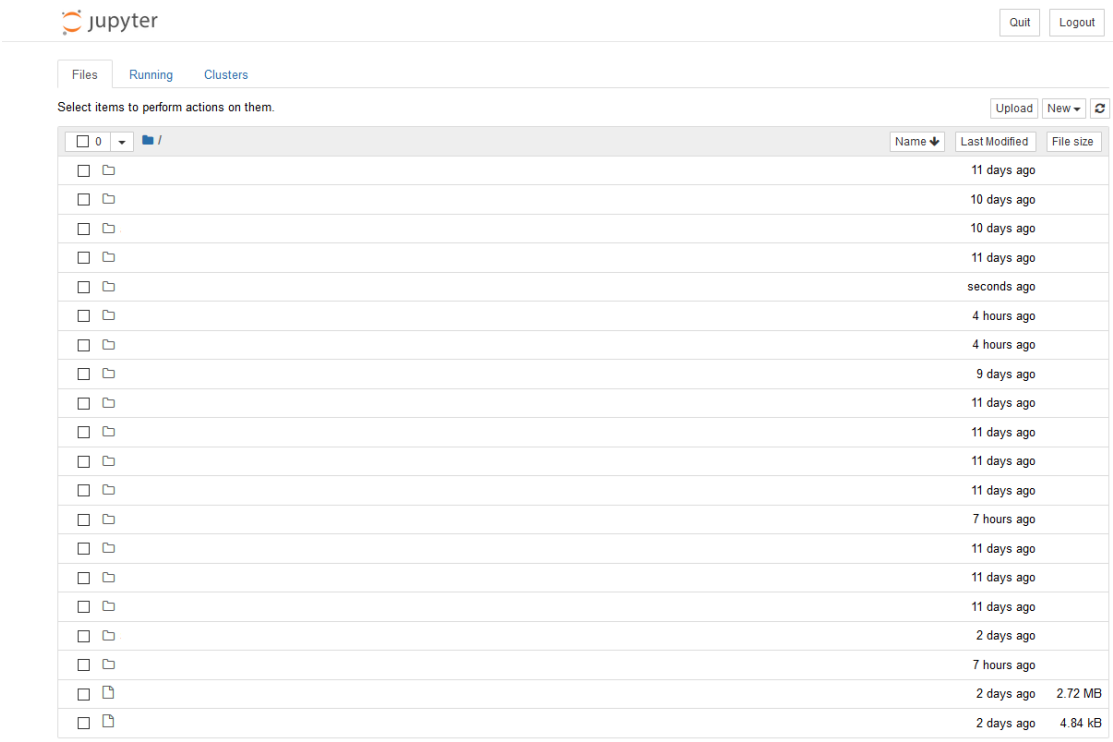


Figure 3.5: Caption

3.2 How to use Jupyter Notebook

3.3 Jupyter Notebooks for PyTherm

3.3.1 Lesson 1 - Preparing Thermodynamic Calculations

3.3.2 Lesson 2 - Performing Thermodynamic Calculations

3.3.3 Lesson 3 - Comparison Functions

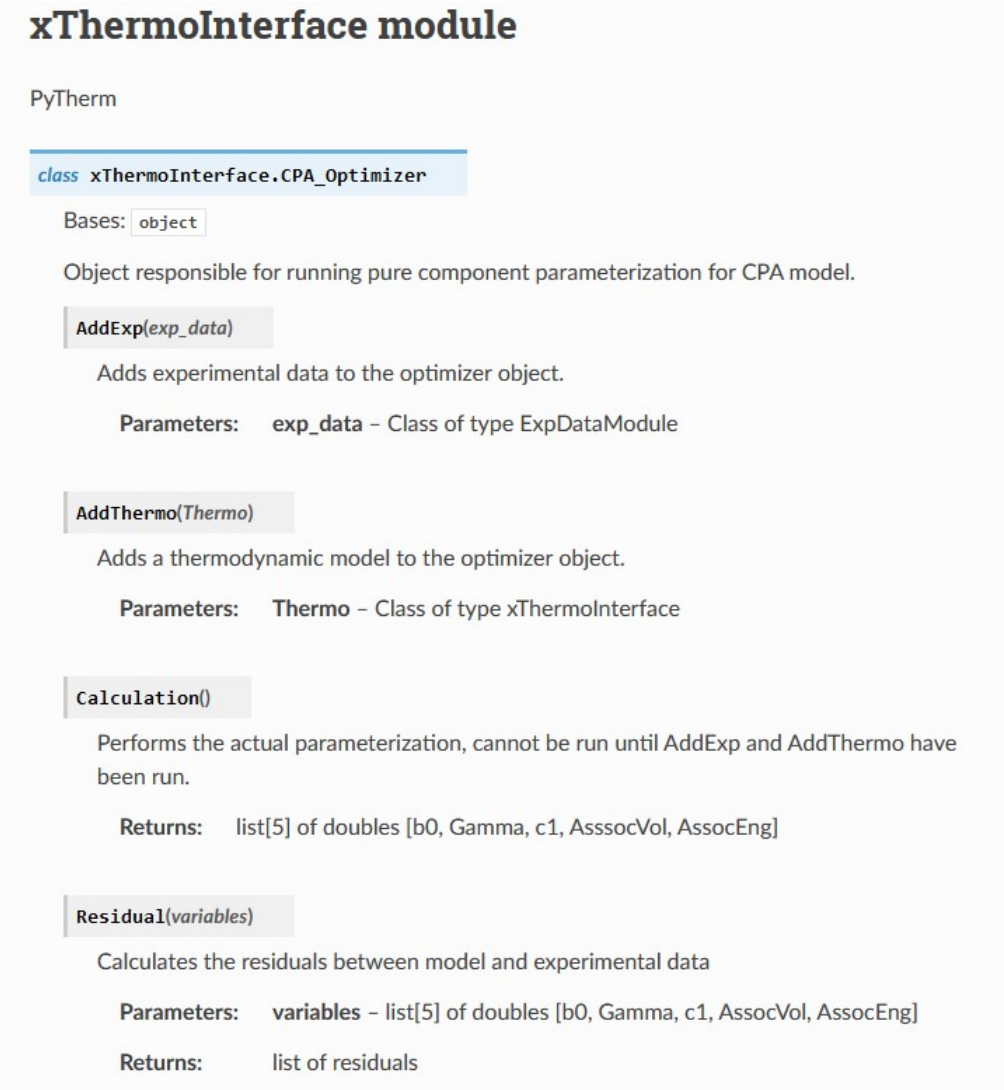
3.3.4 Lesson 4 - Parameter Optimization

4 Module Syntax

The python documentation for the PyTherm module may be found by following the following procedure.

1. Head to the folder containing the downloaded files.
2. Open the shortcut called ”Python Documentation”. Any browser may be used.

Below you will see an example from the documentation page.



xThermoInterface module

PyTherm

class **xThermoInterface.CPA_Optimizer**

Bases: `object`

Object responsible for running pure component parameterization for CPA model.

AddExp(*exp_data*)

Adds experimental data to the optimizer object.

Parameters: **exp_data** – Class of type ExpDataModule

AddThermo(*Thermo*)

Adds a thermodynamic model to the optimizer object.

Parameters: **Thermo** – Class of type xThermoInterface

Calculation()

Performs the actual parameterization, cannot be run until AddExp and AddThermo have been run.

Returns: list[5] of doubles [b0, Gamma, c1, AsssocVol, AssocEng]

Residual(*variables*)

Calculates the residuals between model and experimental data

Parameters: **variables** – list[5] of doubles [b0, Gamma, c1, AssocVol, AssocEng]

Returns: list of residuals

Figure 4.1: Screenshot of the documentation page

A Title