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# **pyZacros Documentation**

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# CONTENTS

<b>1</b>	<b>Contents:</b>	<b>3</b>
	<b>Python Module Index</b>	<b>5</b>
	<b>Index</b>	<b>7</b>



This is the documentation for pyZacros a library to run your favorite KMC code.



## CONTENTS:

## 1.1 Getting started

### 1.1.1 Quick installation

Hello world!

### 1.1.2 First steps

Hello world!

## 1.2 Modules

### 1.2.1 Classes

KMC Class

Settings Class

### 1.2.2 Utility functions

#### find\_utils.py module

Module containing utility functions to find files.

`pyzacros.utils.find_utils.find_file(name, path_to_search)`  
Find a given name file.

`pyzacros.utils.find_utils.find_input_files(engine: str, electronic_package: Optional[str] = None, path: Optional[str] = None) → list`  
Search enigne.yml or engine.yaml input files.

If none, engine standard input files will be searched. :return: A list of input files. :rtype : list.

`pyzacros.utils.find_utils.find_path_to_engine(settings: pyzacros.classes.KMCSettings.KMCSettings) → tuple`

Find the path to the KMC engine using the sett.KMCEngine.path.

**Parm settings** KMCSettings object with the main settings of the KMC calculation.

**Return path\_to\_engine** The path to the engine.

**Rtype path\_to\_engine** str

## pyzacros.utils.io\_utils module

Module containing utilities to read/write data.

`pyzacros.utils.io_utils.read_input_data(engine: str, electronic_package: Optional[str] = None, path: Optional[str] = None)`

Search input files. In increasing herarchical order.

- Read engine standard input.
- Read ab-initio output input.
- Read formatted yaml or hdf5 files.

**Returns** instantiation of PLAMS-like settings according for the input files read.

`pyzacros.utils.io_utils.write_kmc_input_files(engine: str)`

Write KMC input files.

**Parm engine** Name of the engine

## Module contents

#Module contents #————— #.. automodule:: pyzacros # :members: # :undoc-members: # :show-inheritance:



## PYTHON MODULE INDEX

### p

`pyzacros.utils`, 4

`pyzacros.utils.find_utils`, 3

`pyzacros.utils.io_utils`, 4



## INDEX

### F

`find_file()` (in module `pyzacros.utils.find_utils`), 3  
`find_input_files()` (in module `pyzacros.utils.find_utils`), 3  
`find_path_to_engine()` (in module `pyzacros.utils.find_utils`), 3

### M

module  
    `pyzacros.utils`, 4  
    `pyzacros.utils.find_utils`, 3  
    `pyzacros.utils.io_utils`, 4

### P

`pyzacros.utils`  
    module, 4  
`pyzacros.utils.find_utils`  
    module, 3  
`pyzacros.utils.io_utils`  
    module, 4

### R

`read_input_data()` (in module `pyzacros.utils.io_utils`),  
4

### W

`write_kmc_input_files()` (in module `pyzacros.utils.io_utils`), 4