POLITECNICO MILANO 1863

DIPARTIMENTO DI ENERGIA

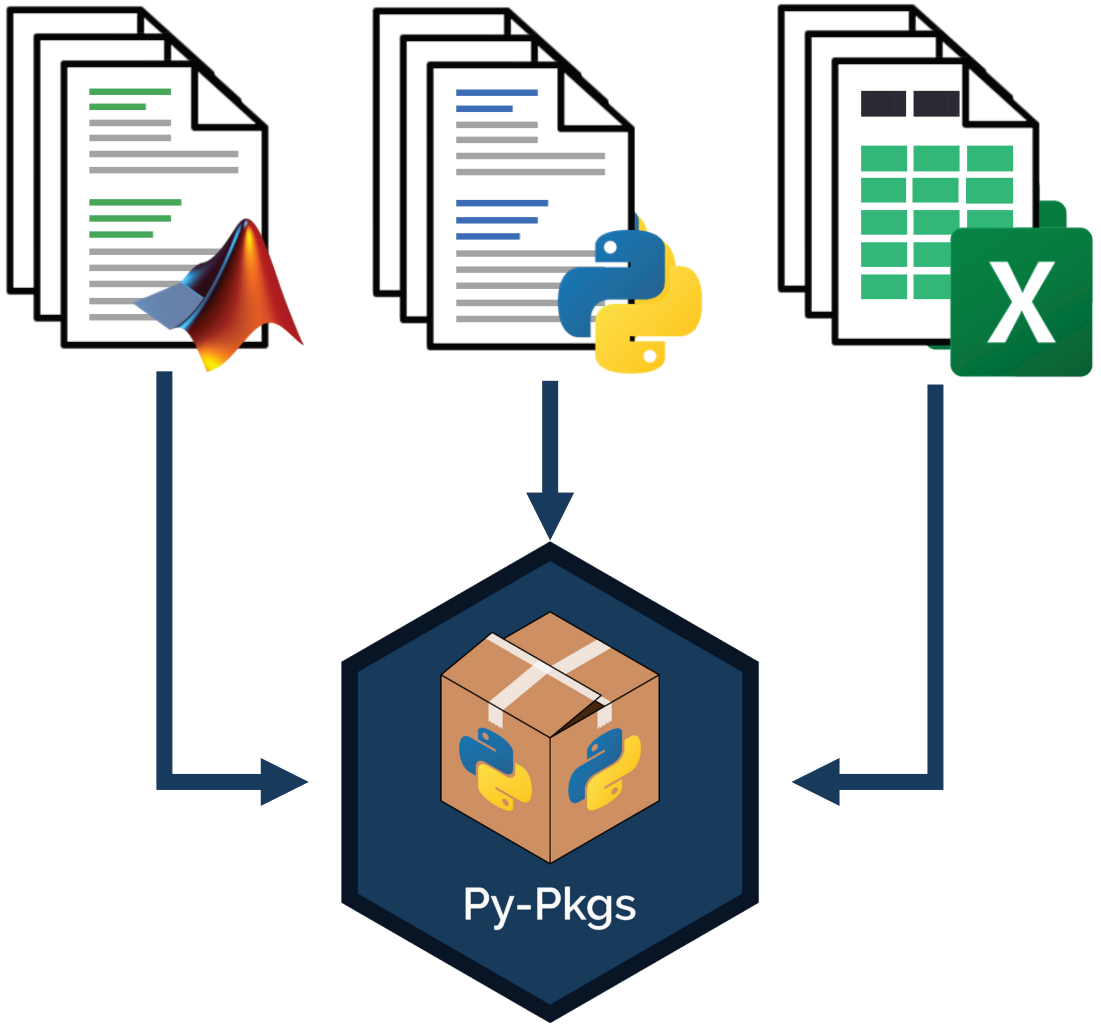
LibICE-post: User guide

Post-processing of experimental and numerical data for ICE applications

Federico Ramognino

Why libICEpost…?

- **No common methodology** was present for processing of results (experimental or CFD simulations), leading to:
  - Redundancy and duplication of code
  - Multiple codes and software
  - Risk of errors
  - Loss of efficiency and knowledge
- Need for a **standardized framework** to be shared within the research group
- Organizing all methodologies in a single **python package**
- …why **python?**
  - ✓ Free (no licence required)
  - ✓ Strong community (many packages available)
  - ✓ Easy to use
  - ✓ Versatile
  - ✓ Not OS-dependent



What is inside `libICEpost`

- **Scope of the package:**
  - ➢ Implementation **methodologies** for pre/post-processing of data from internal combustion engines applications

- **Main features:**
  - ✓ Modeling of mixtures, with their thermodynamic properties
  - ✓ Modeling of internal combustion engines for processing heat release rate and heat transfer from pressure traces
  - ✓ Input/output interfaces for processing OpenFOAM results

- **Requirements**: python>=3.11

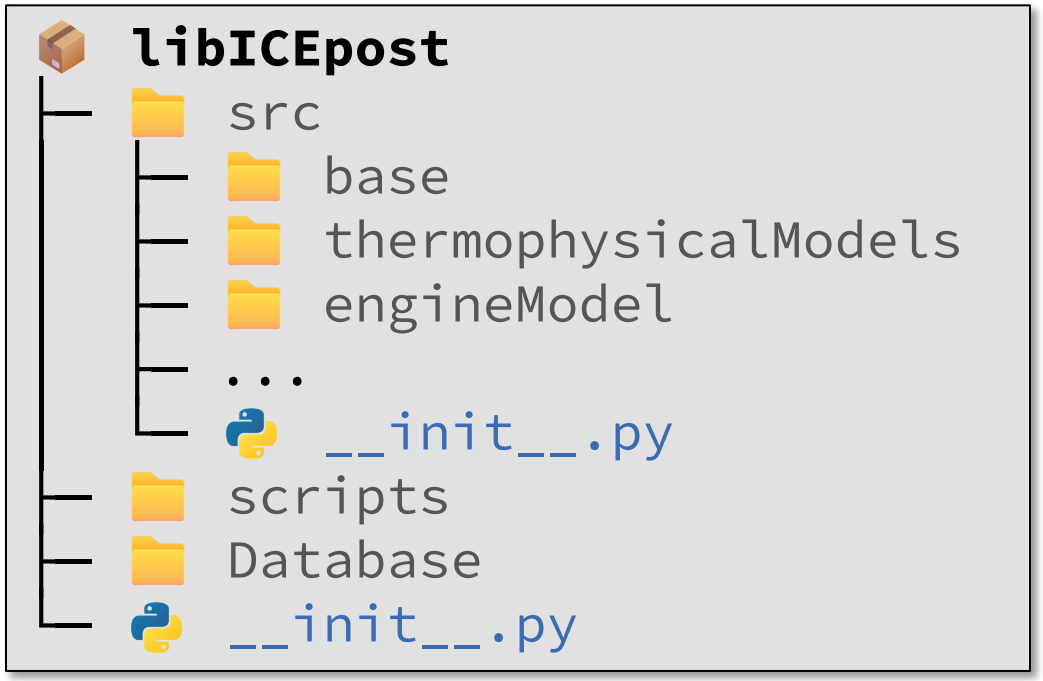
```
user@localhost: ~

(base) user@localhost:~$ pip install libICEpost
```

PyPI: https://pypi.org/project/libICEpost/

GitHub: https://github.com/RamogninoF/LibICE-post

Structure of the package

- **Three** main **subpackages**:



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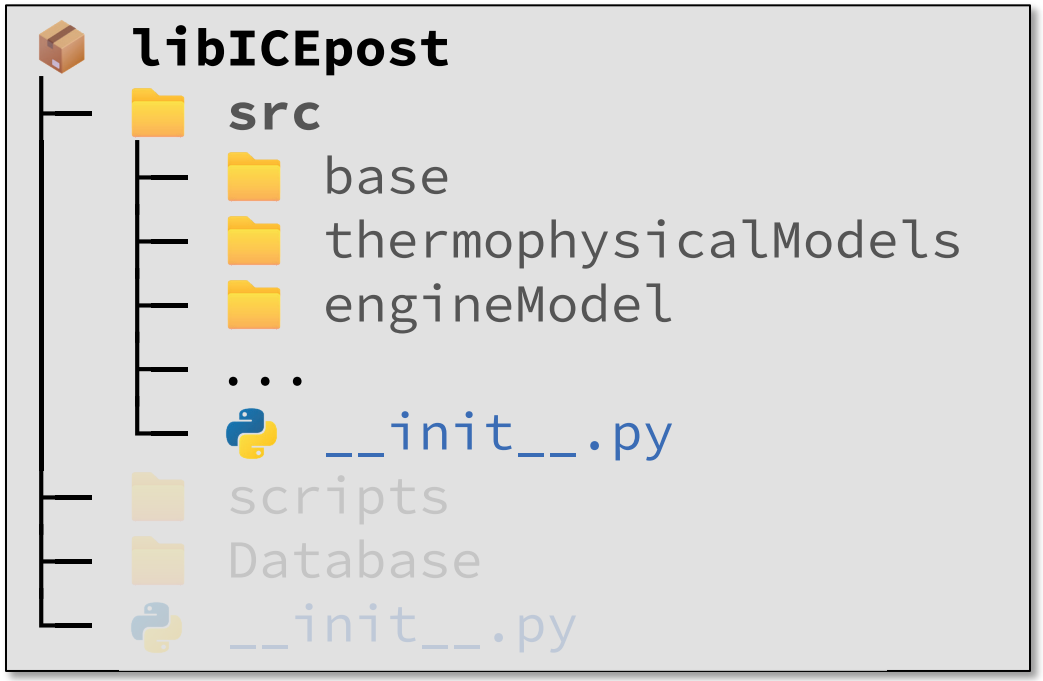
  - **`src`** – Core of the library, contains all **functions** and **classes**. Major groups are:
    - `base` – generic-use classes and functions
    - `thermophysicalModels` – modeling of chemistry and thermophysical properties of mixtures
    - `engineModel` – models for description of ICE



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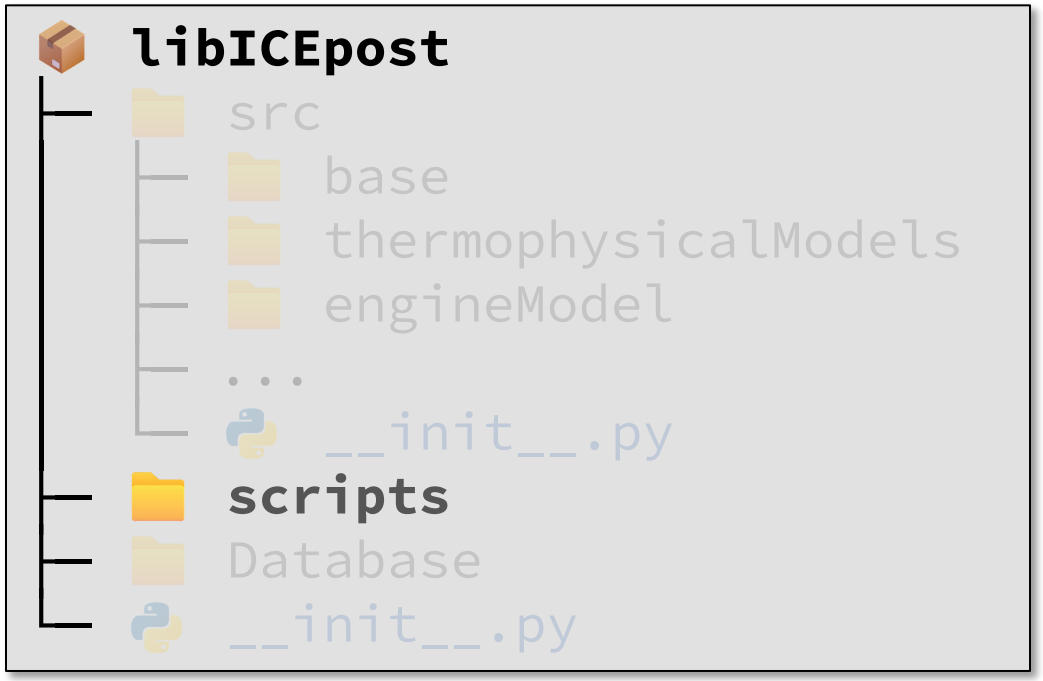
  - **`scripts`** – Contains **executable scripts**, where automated workflows can be implemented



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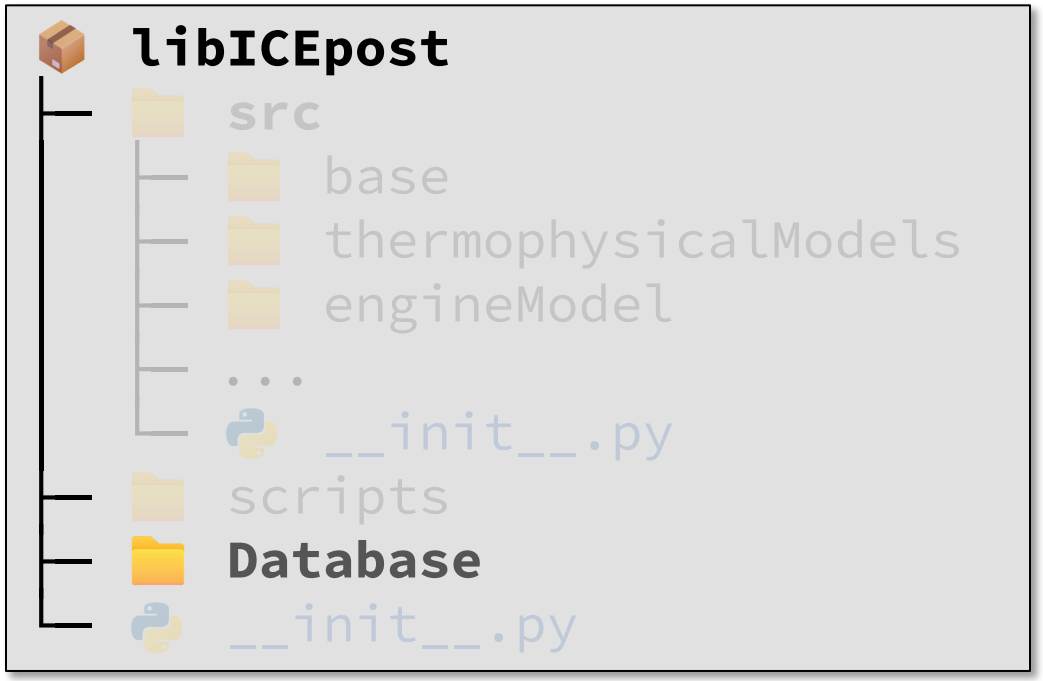
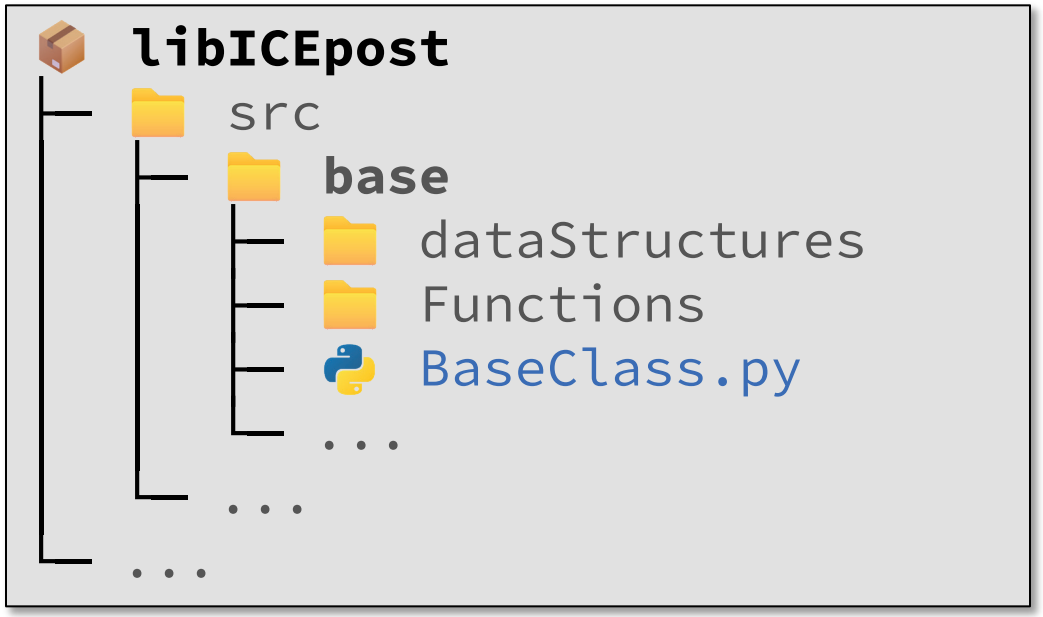
  - `scripts` – Contains **executable scripts**, where automated workflows can be implemented
  - **`Database`** – A built-in database with useful data (periodic table, molecules, fuels, thermophysical properties, etc.)



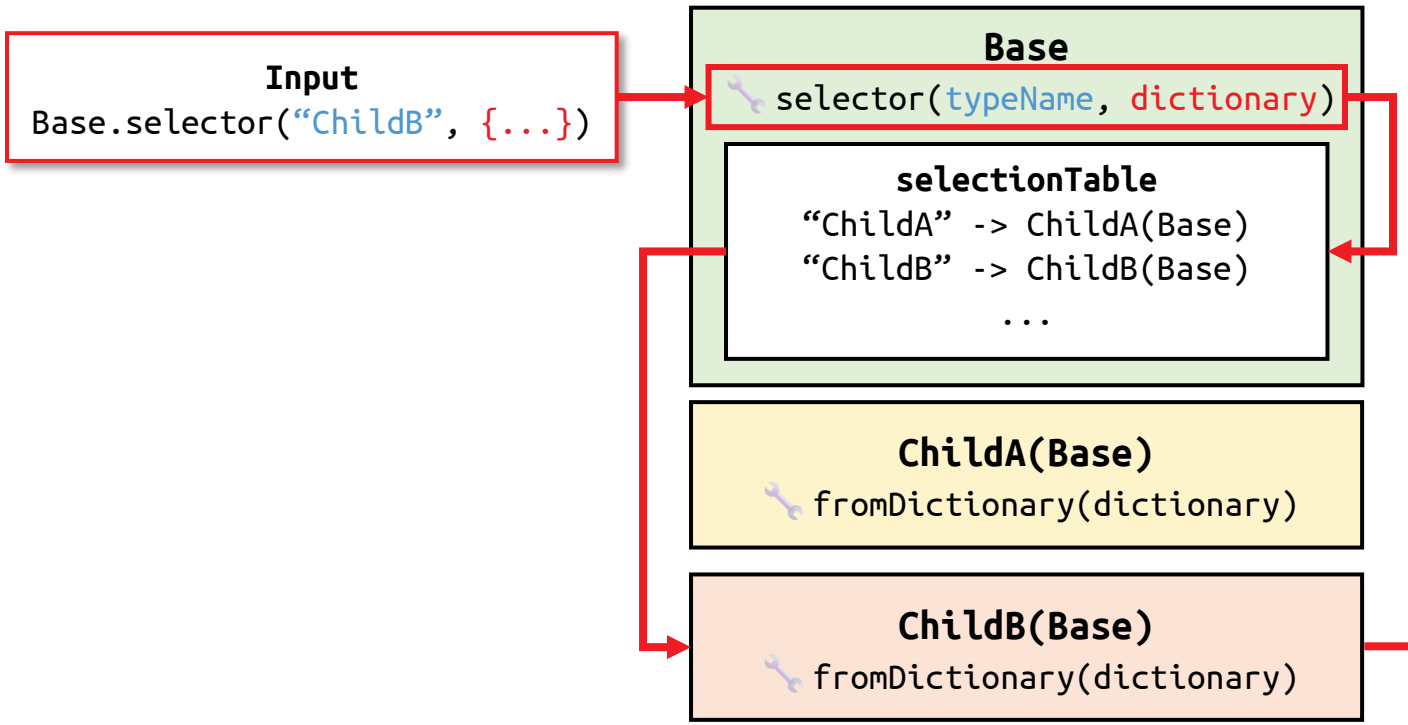
libICEpost.src.base

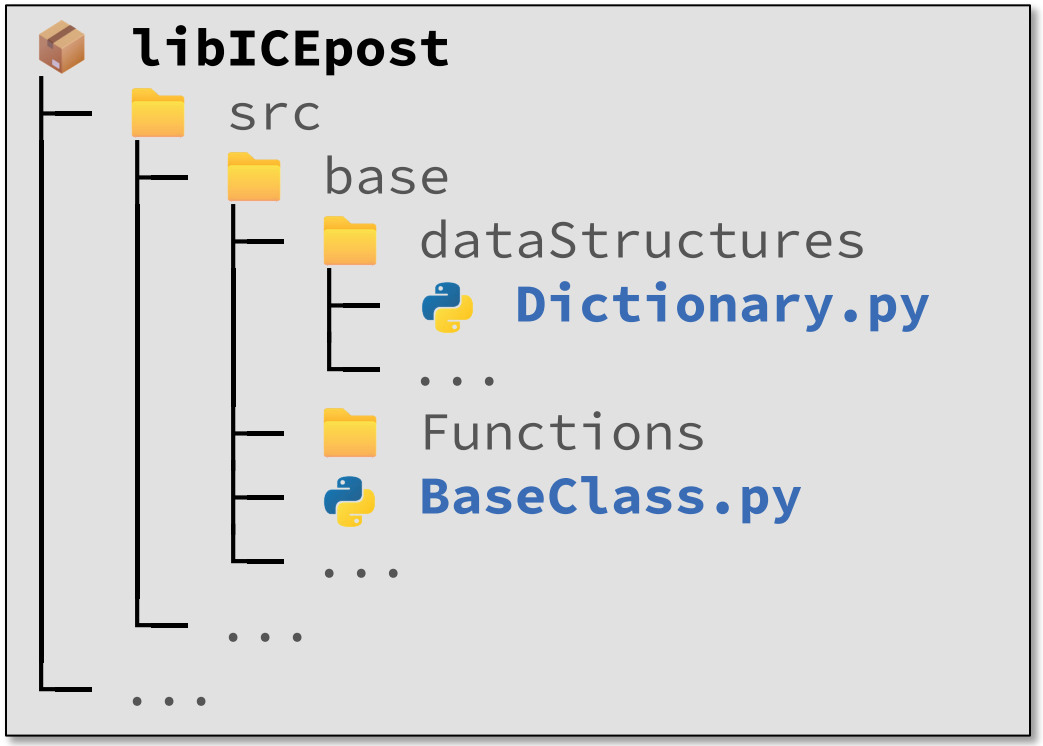
- Generic-use **classes** (data-structures, signal filters, etc.) and **functions** (I/O, OpenFOAM interfaces, etc.)



Input/Output and run-time selection

- Generic-use **classes** (data-structures, signal filters, etc.) and **functions** (I/O, OpenFOAM interfaces, etc.)
- Implementation of **I/O** and **run-time selection** of models following OpenFOAM rationale





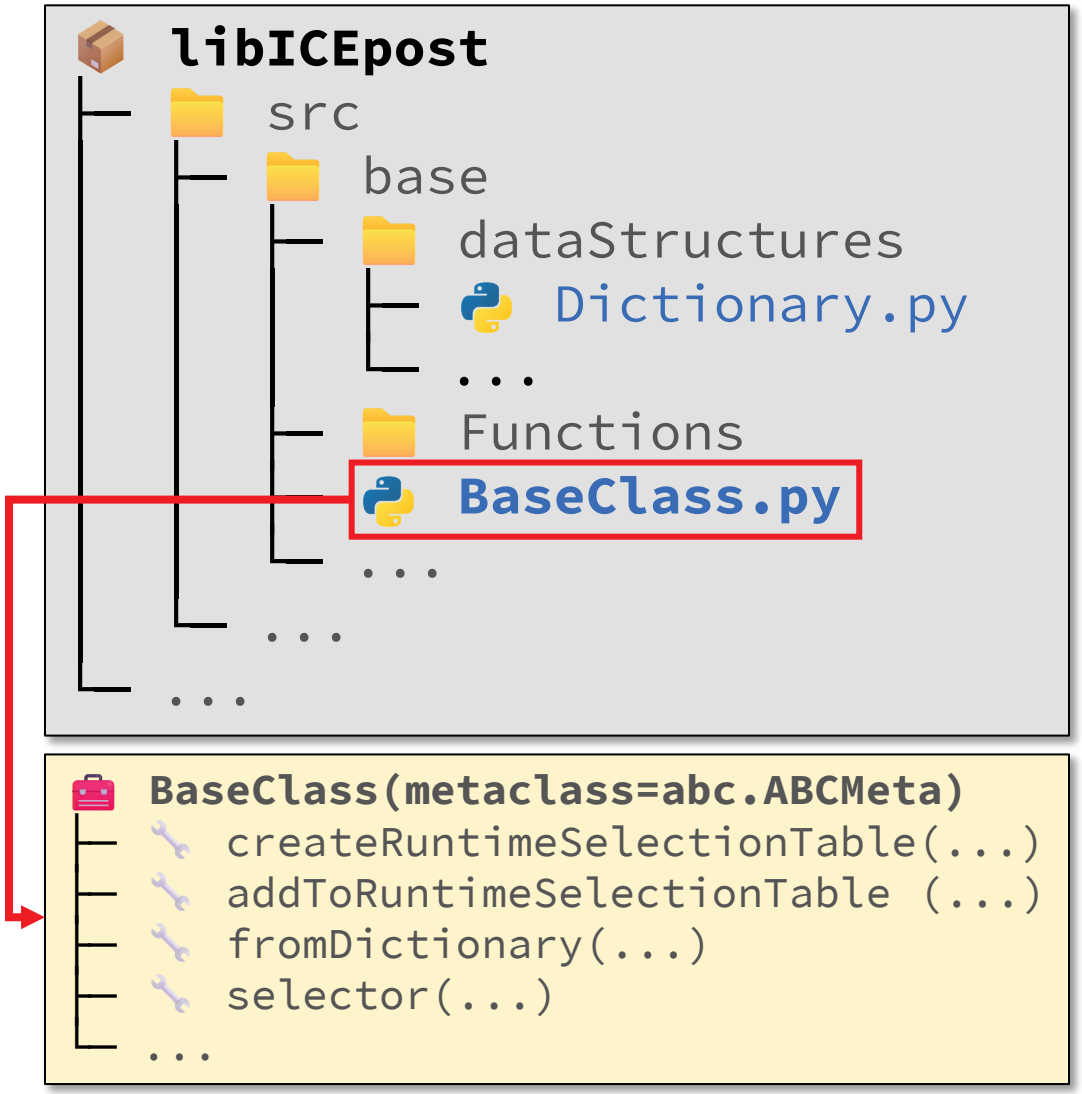
Run-time selection – BaseClass

- **BaseClass** – Virtual Base Class with implementation of run-time selection for handling model choice
  - ➢ Used to give abstract-base-class functionalities to classes defining the structure of models

libICEpost\src\thermophysicalModels\specie\thermo\Thermo\Thermo.py

```
1  """
2  Base class for computati                    cie (cp, cv, ...)
3  """
4  class Thermo(BaseClass):
5      @abstractmethod
6      def cp(self, p, T): # ...
7      # ...
8
9  Thermo.createRuntimeSelectionTable() #Creating of the selection table for Thermo
```

Abstract class defining the structure of the model **inheriting from BaseClass**



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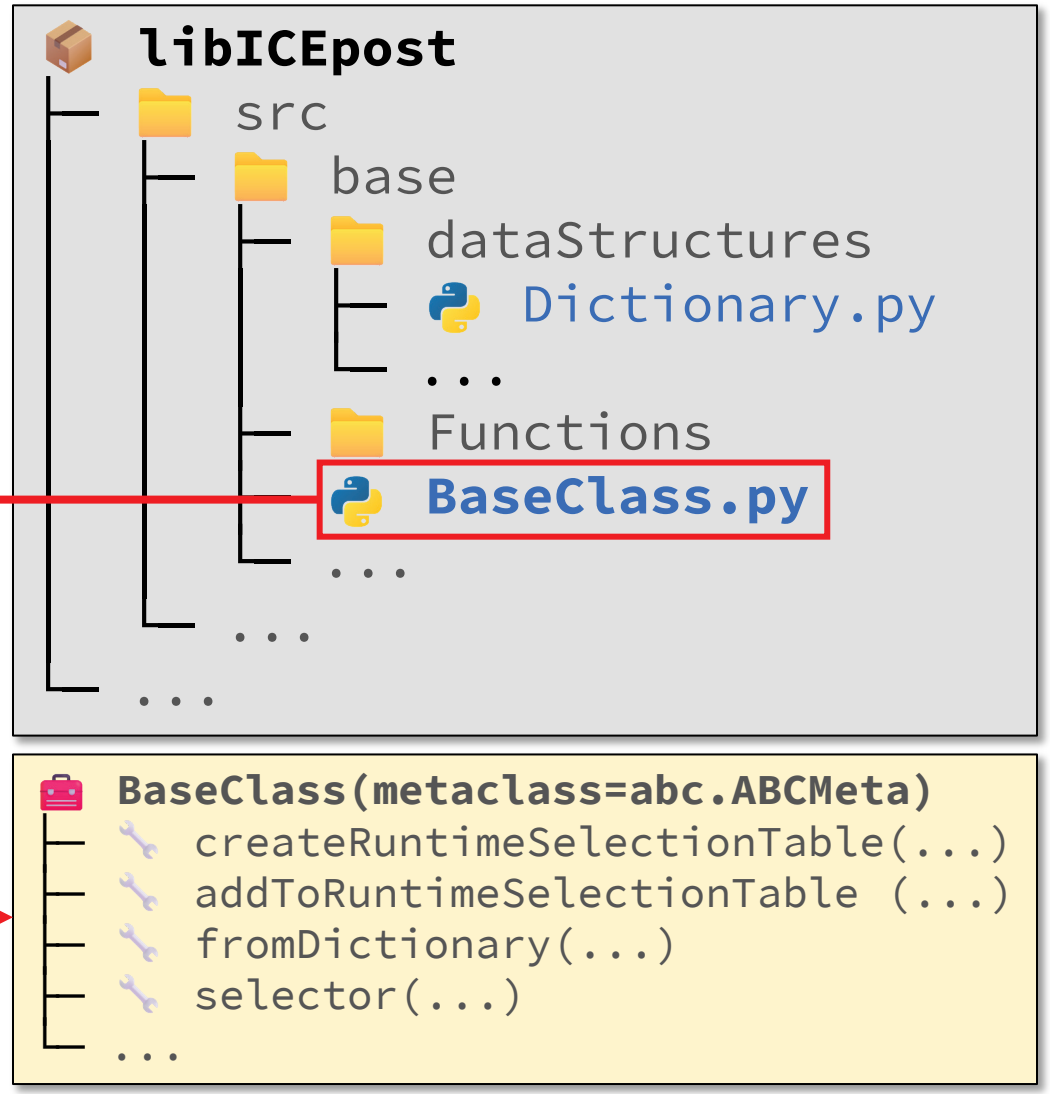
Virtual methods to be overwritten in child classes



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  - **Creation of selection-table** for the **VBC** defining the common structure of the specific model

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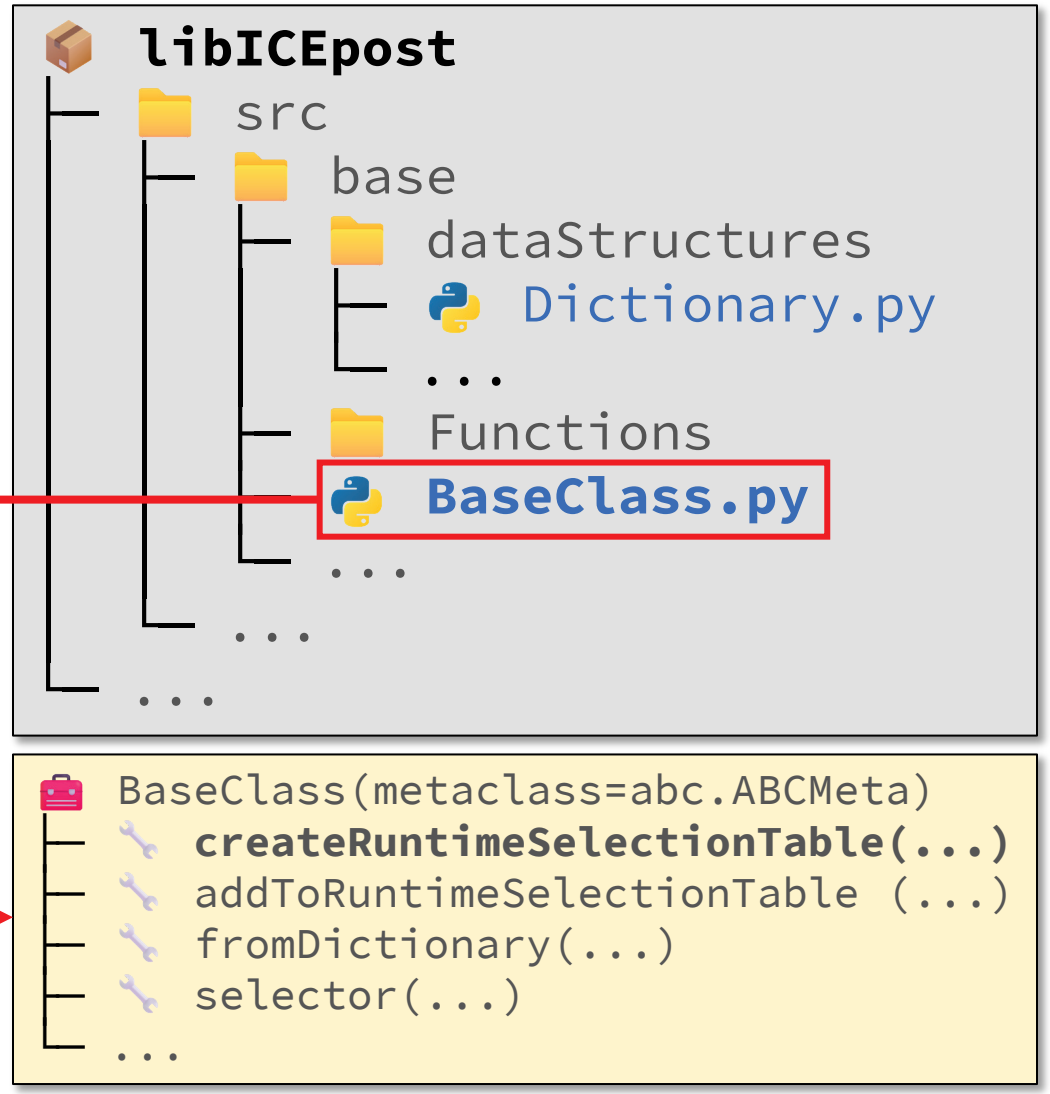
Creation of the **selection table** for class Thermo



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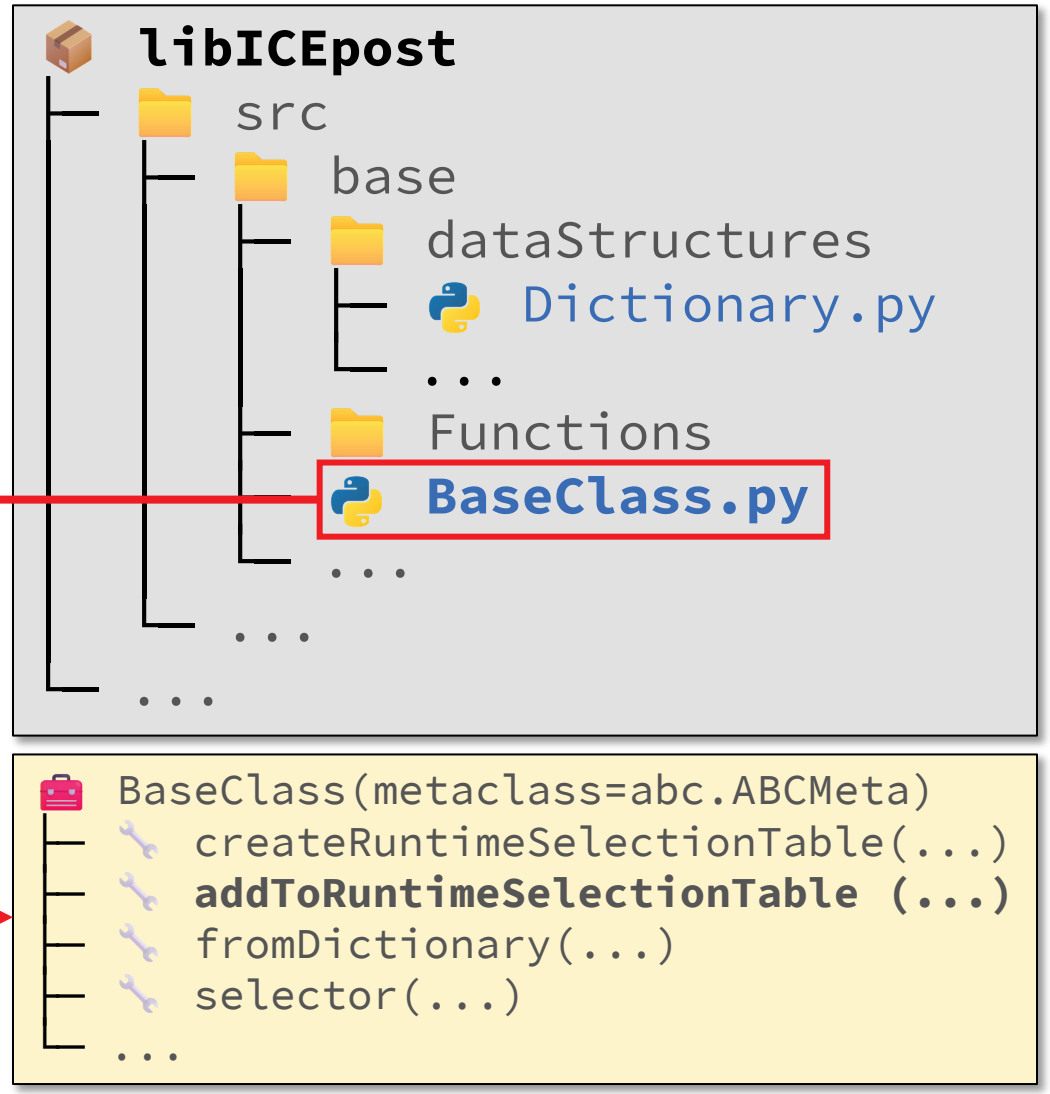

libICEpost\src\thermophysicalModels\specie\thermo\Thermo\janaf7.py

```python
from .Thermo import Thermo      #Importing the (virtual) base class

# Computation of thermophysical                    ient polynomials.
class janaf7(Thermo):
    @classmethod
    def fromDictionary(cls,dictionary): #...
    @classmethod
    def cp(self, p, T): #...

Thermo.addToRuntimeSelectionTable(janaf7) #Adding janaf7 to the table of Thermo
```

Inheriting from abstract class Thermo

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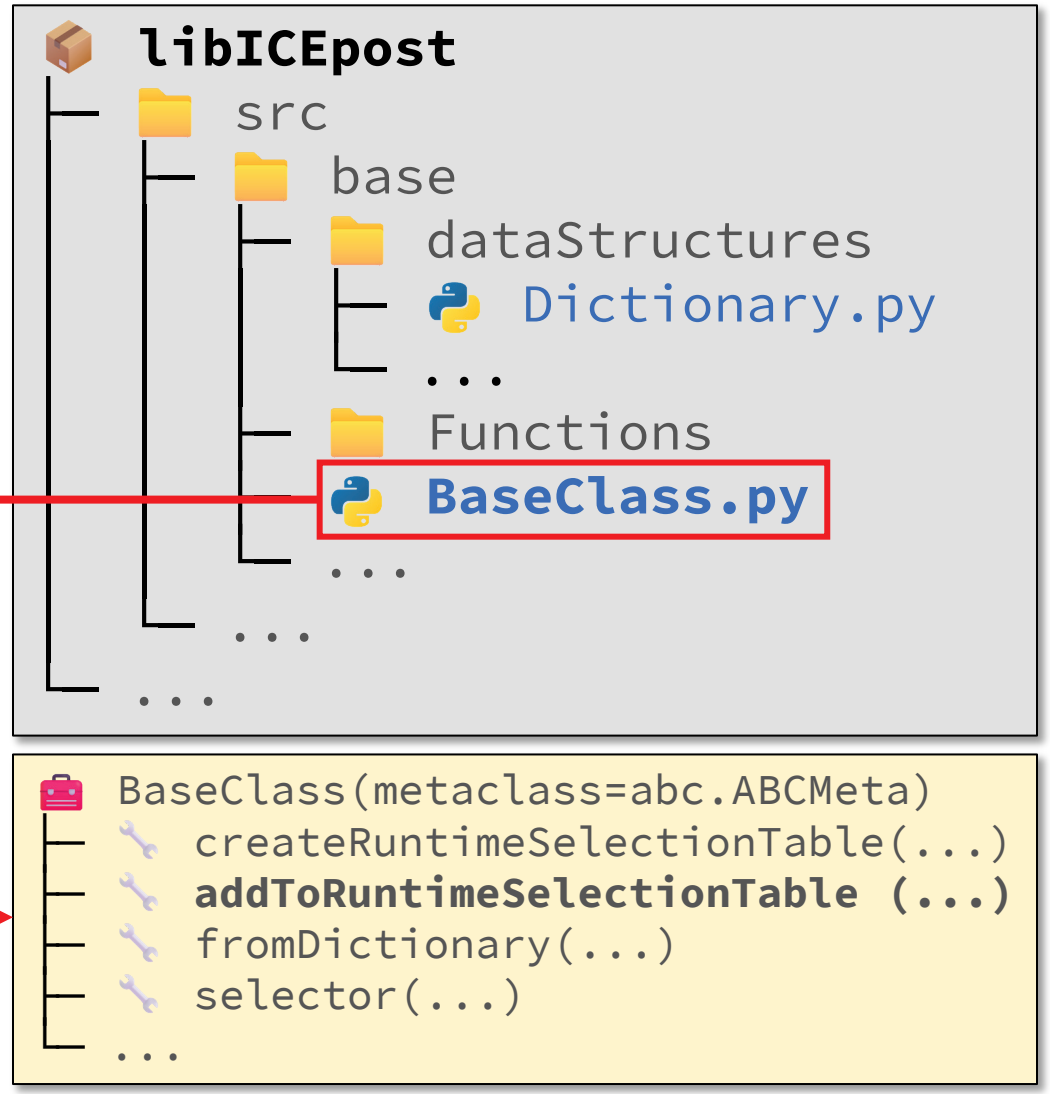

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Implementation of virtual methods

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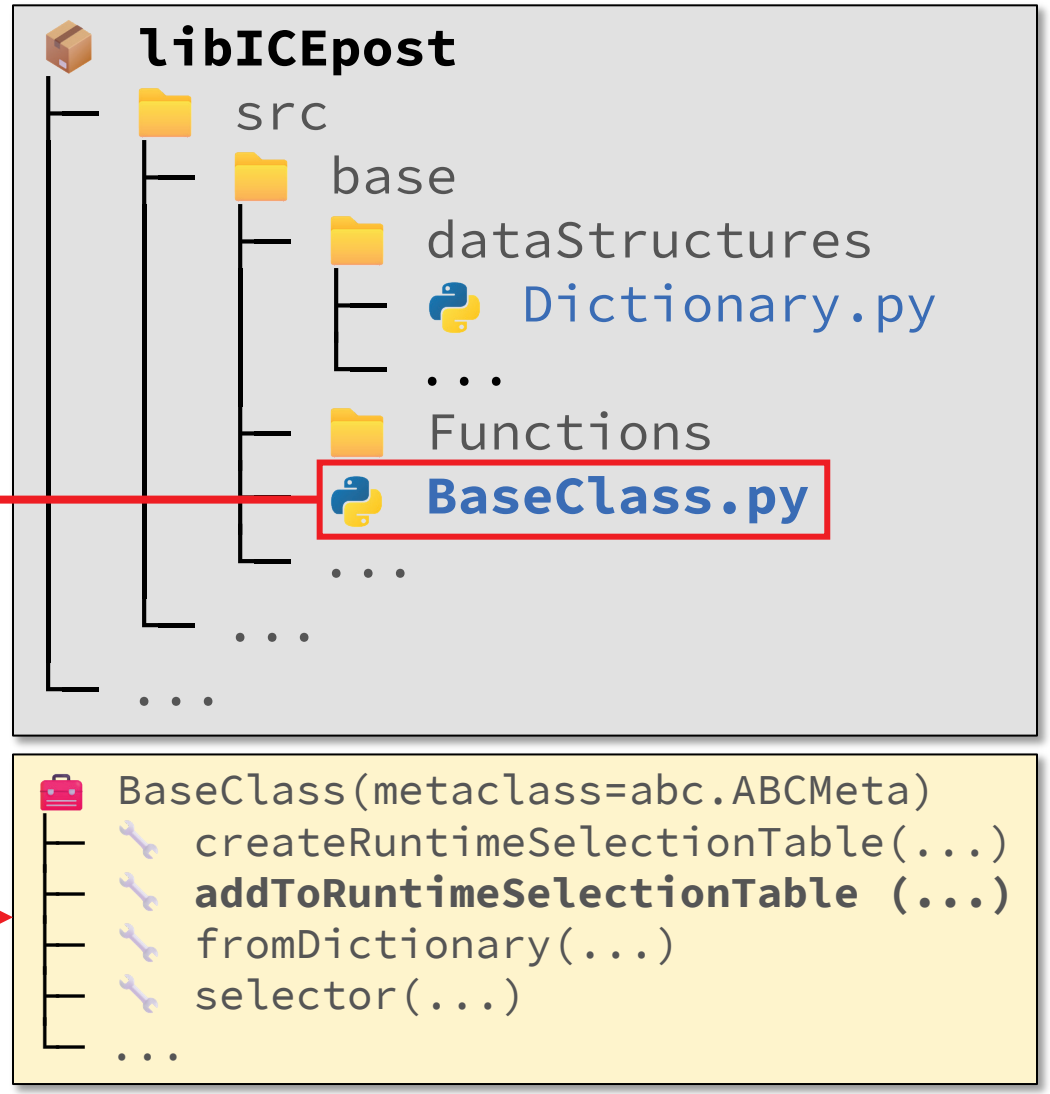

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Adding janaf7 to the selection table of Thermo

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  - Defining a **`fromDictionary` method**, which is used during the run-time selection for **construction from a dictionary**

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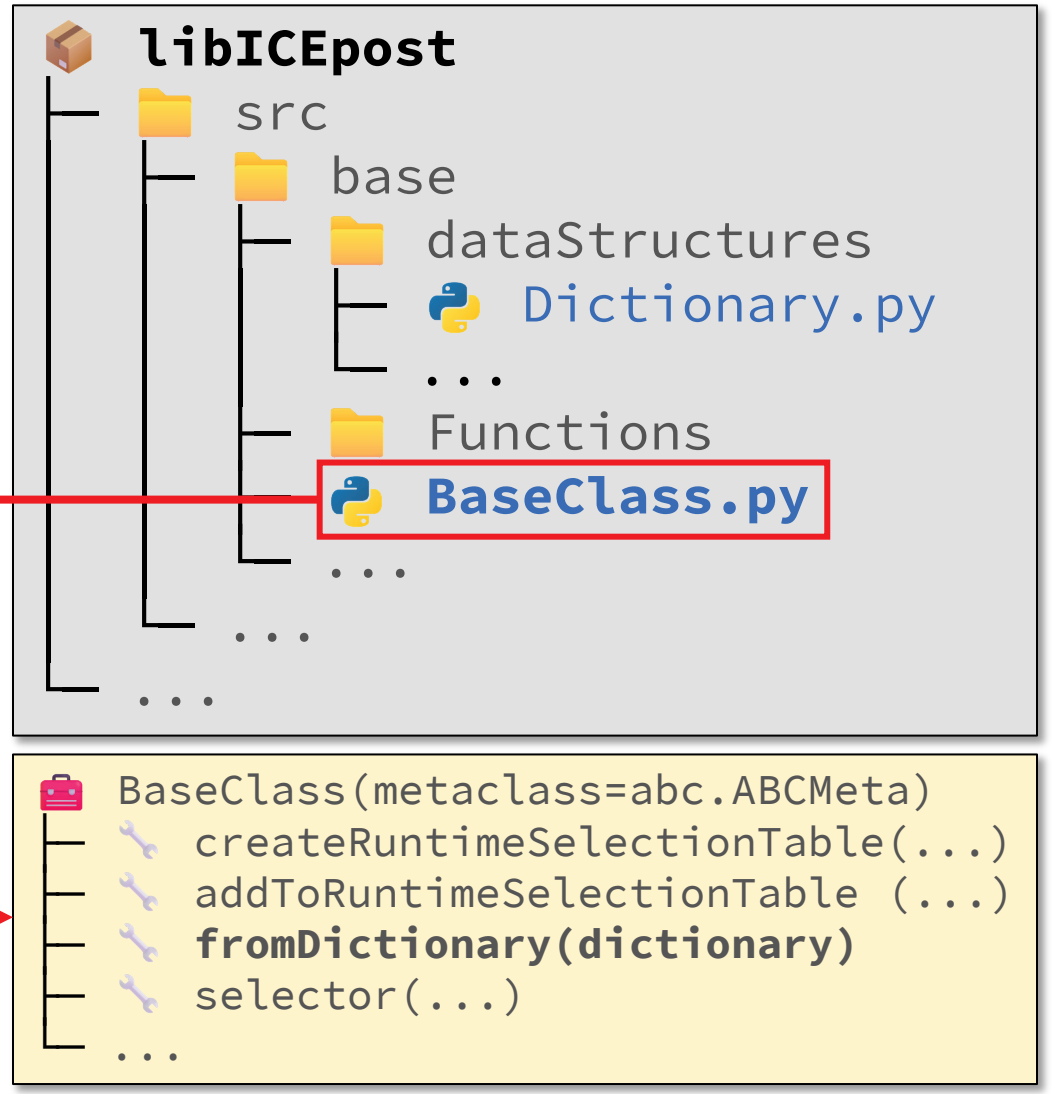
Method for construction from a dictionary entry



Run-time selection – `BaseClass`

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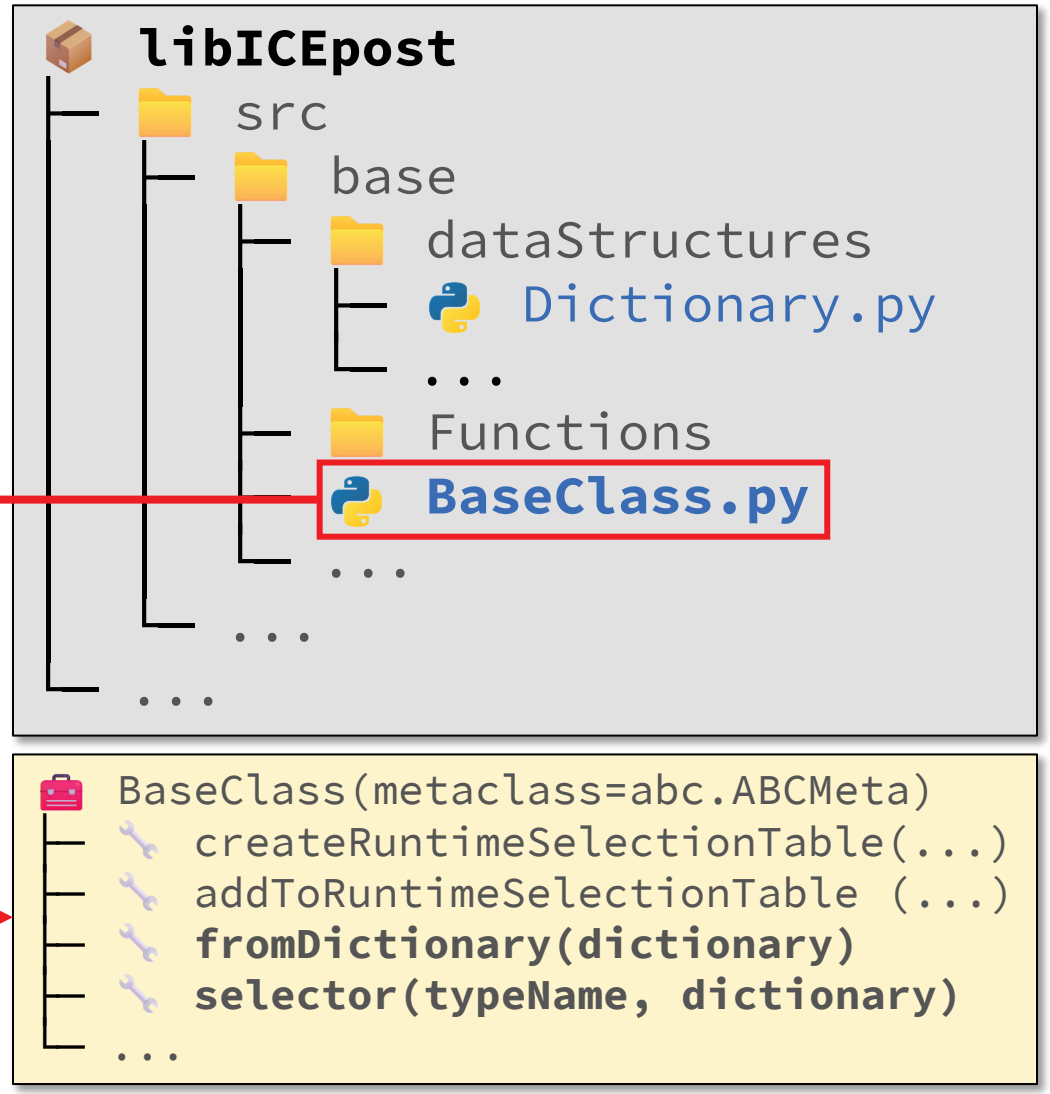
  - Selection of the model with a **common interface** (`selector`), using the **model's name** and a **dictionary**, which is fed to the `fromDictionary` `classmethod` of the required child-class

test.py

```python
from libICEpost.thermophysicalModels.specie.thermo.Thermo.Thermo import Thermo #Loading Thermo
dictionary = {
    "Rgas":     287, # J/kgK
    "gamma":    1.4, # cp/cv ratio
}
thermo = Thermo.selector("constantCp", dictionary) #Construction from selector
```

Construction of **constantCp** class from dictionary



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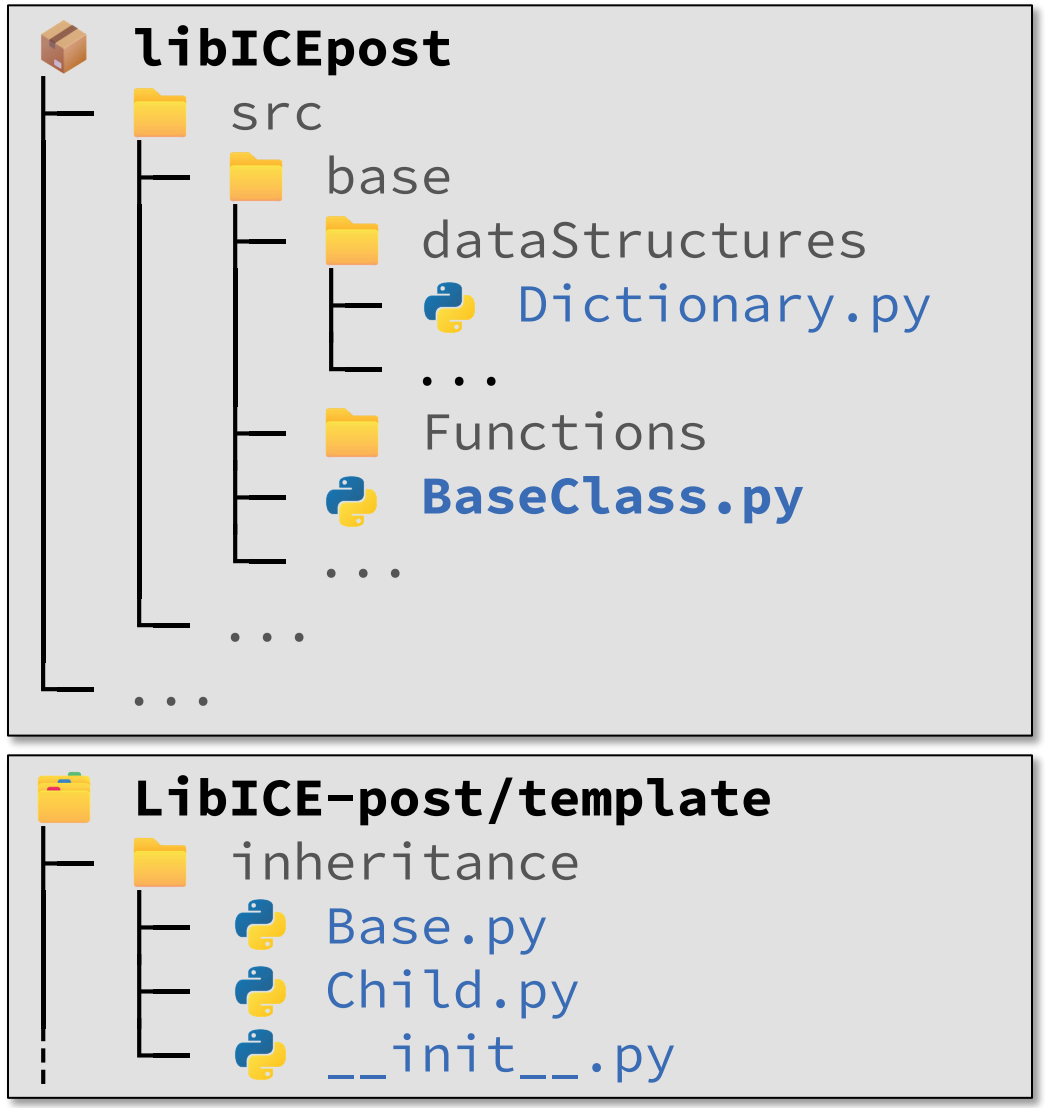
  - **Template of class inheritance structure** can be found in the `templates/inheritance/` folder of the GitHub repository



Input/output – Dictionary

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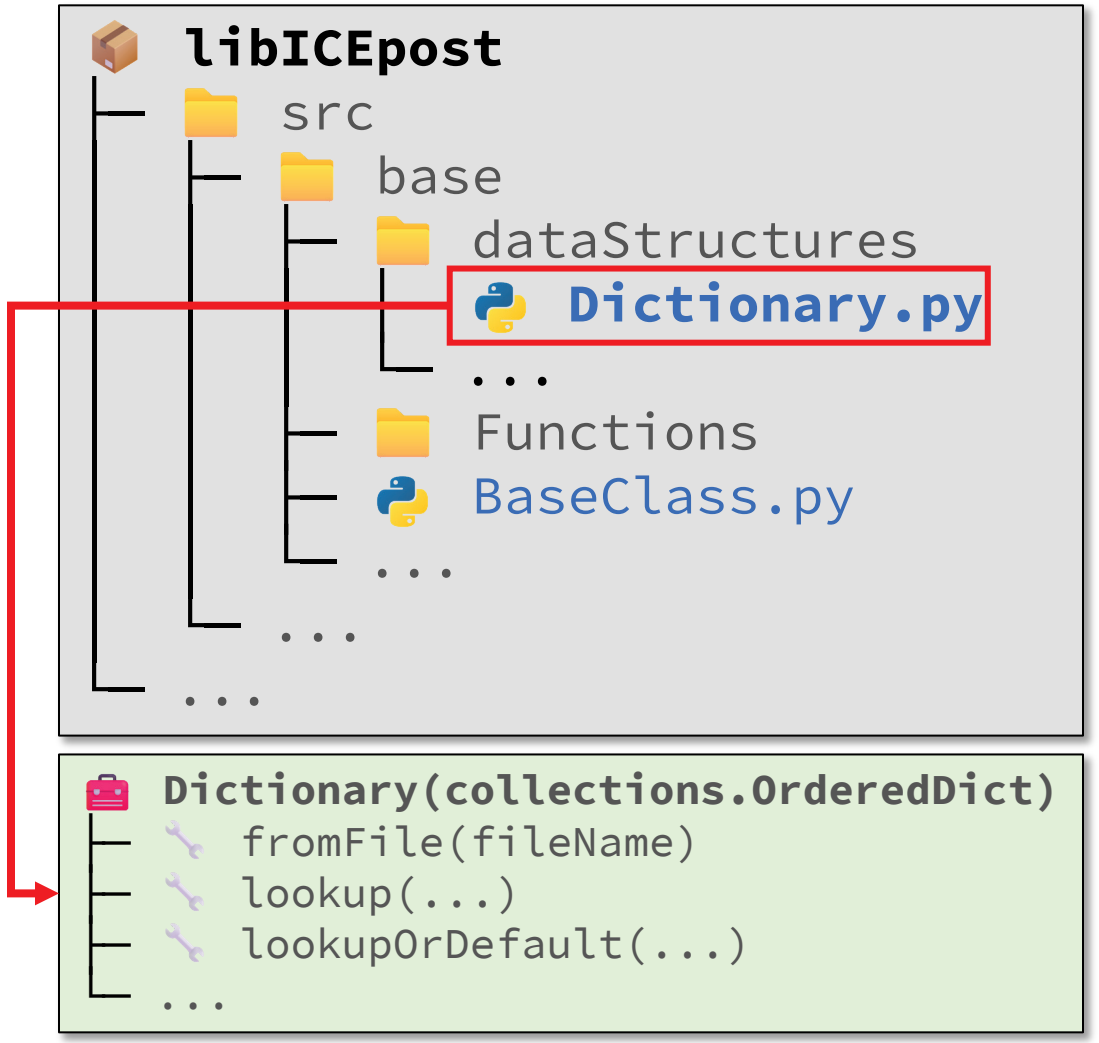
- **Dictionary** – Ordered dictionary embedding useful **I/O and access functionalities**



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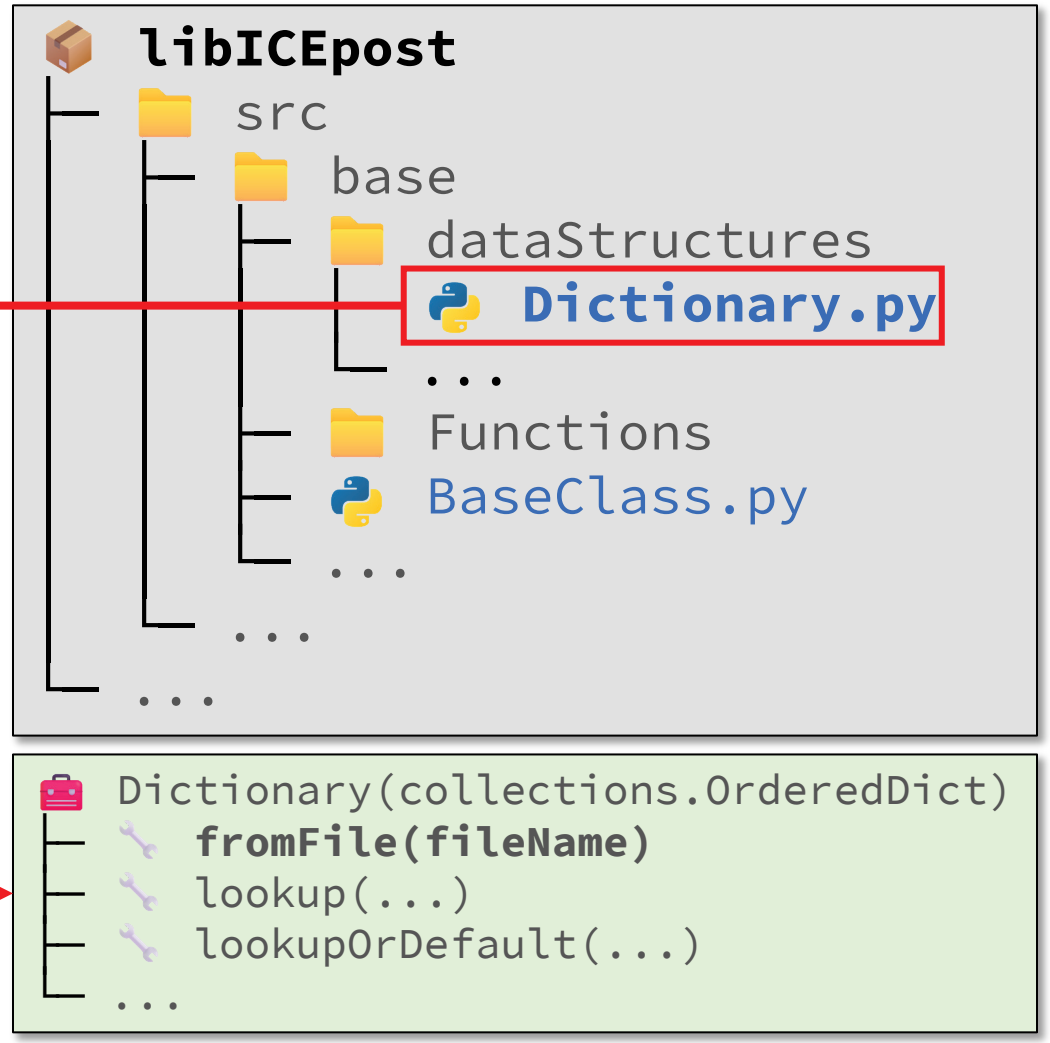
- **Dictionary** – Ordered dictionary embedding useful **I/O and access functionalities**
  - ➢ fromFile: load information **from a python file**. The **file is executed** and all local variables are stored in the dictionary

testDictionary/inputDictionary.py

```
1  #This is a string
2  myString = "a string"
3
4  # This is py
5  pi = 3.1415
```

user@localhost: ~

```
>>> from libICEpost.src.base.dataStructures.Dictionary import Dictionary
>>> dictionary = Dictionary.fromFile("./inputDictionary.py")
>>> print(dictionary)
Dictionary([('myString', 'a string'), ('pi', 3.1415)])
>>> dictionary.lookup("pi")
3.1415
>>> dictionary.lookupOrDefault("g", 9.81)
9.81
```



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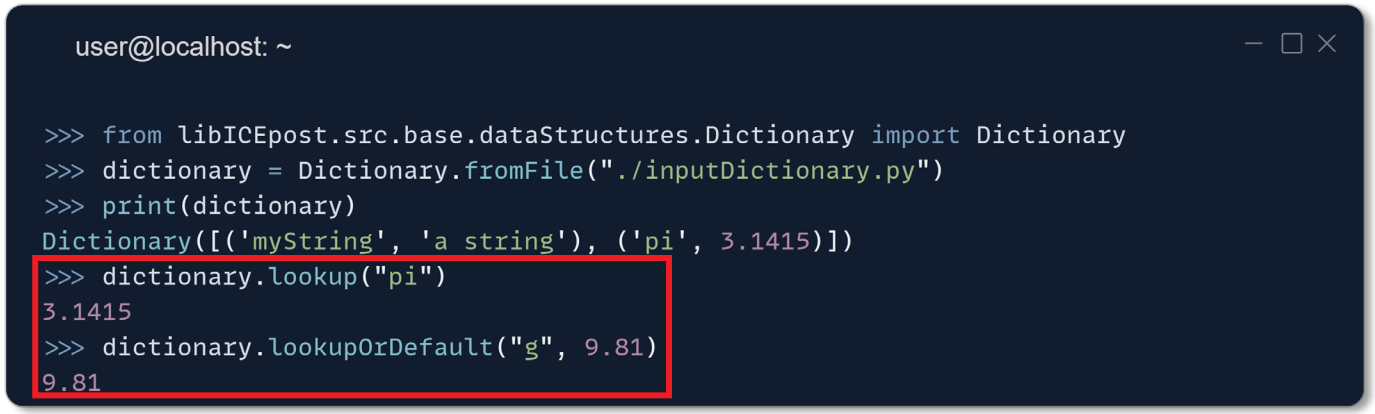
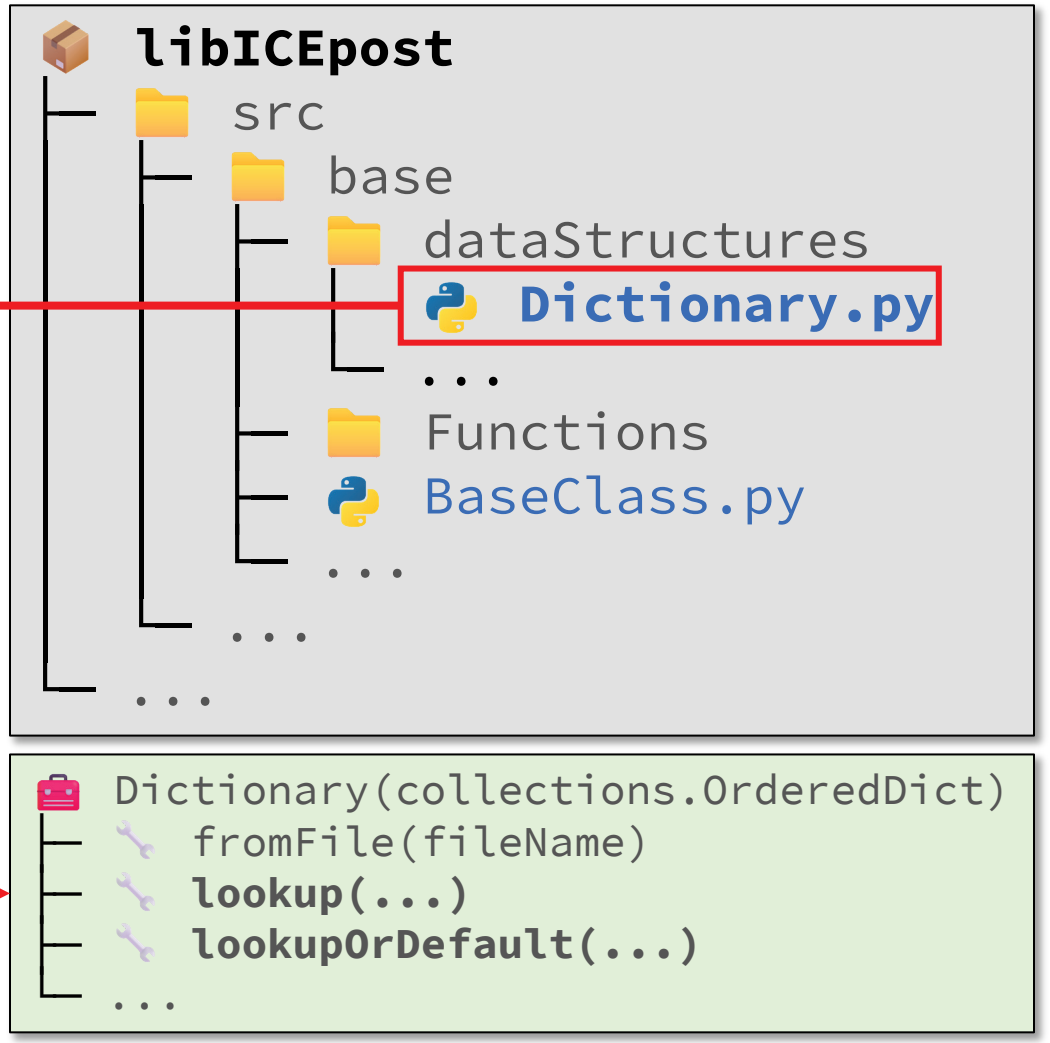
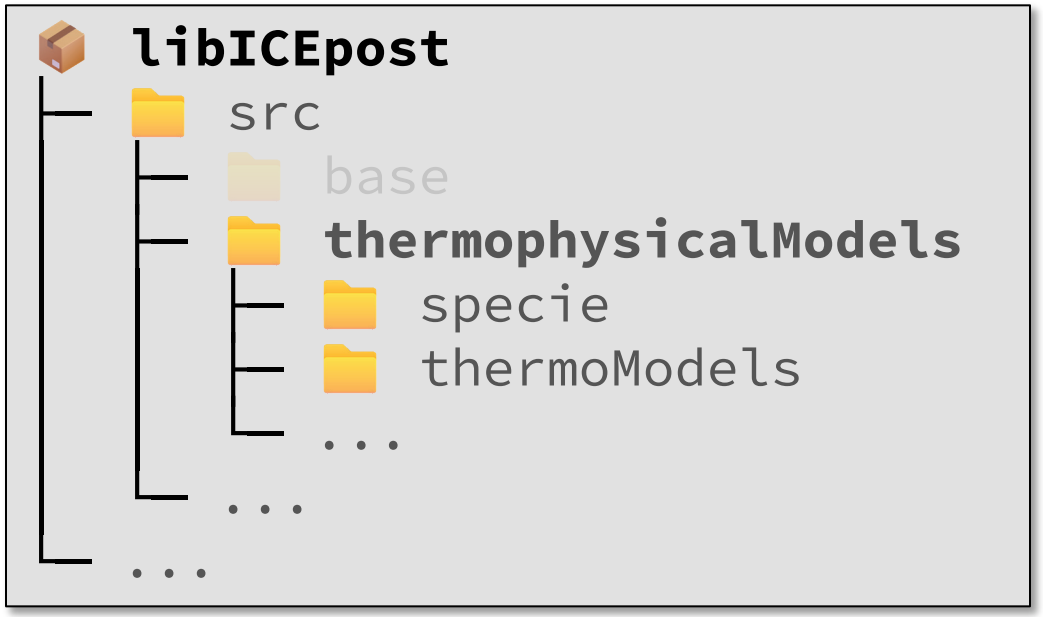
  - fromFile: load information **from a python file**. The **file is executed** and all local variables are stored in the dictionary
  - Convenient **access functions** consistent with OpenFOAM wording, with convenient type-checking and error handling





libICEpost.src.themophysicalModels

- Contains classes and functions for **modeling of chemistry** and **thermophysical properties** of mixtures



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- **Main subpackages**:
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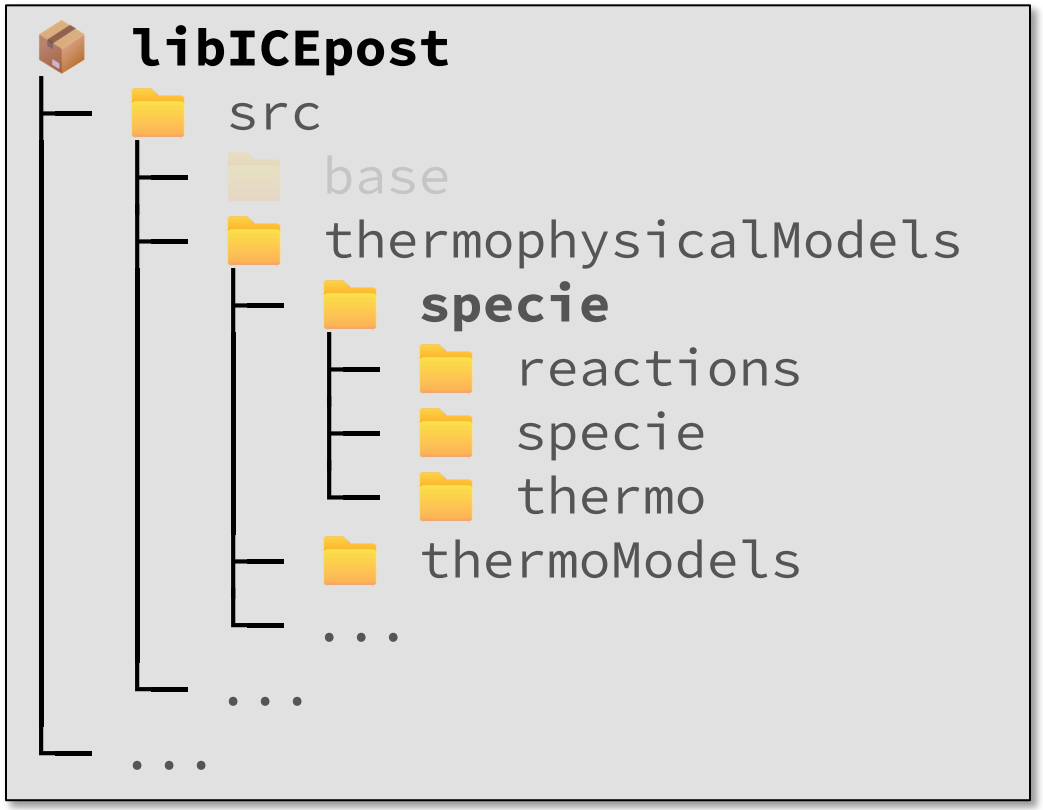

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- **Main subpackages**:
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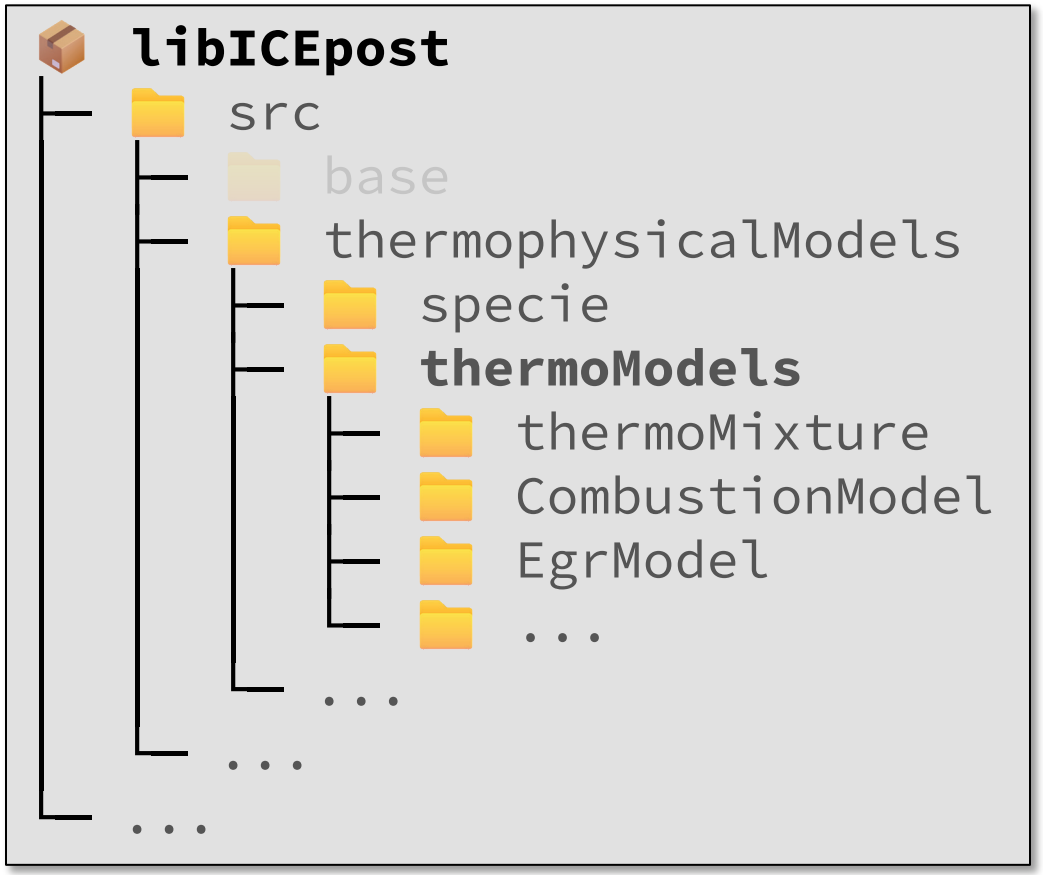
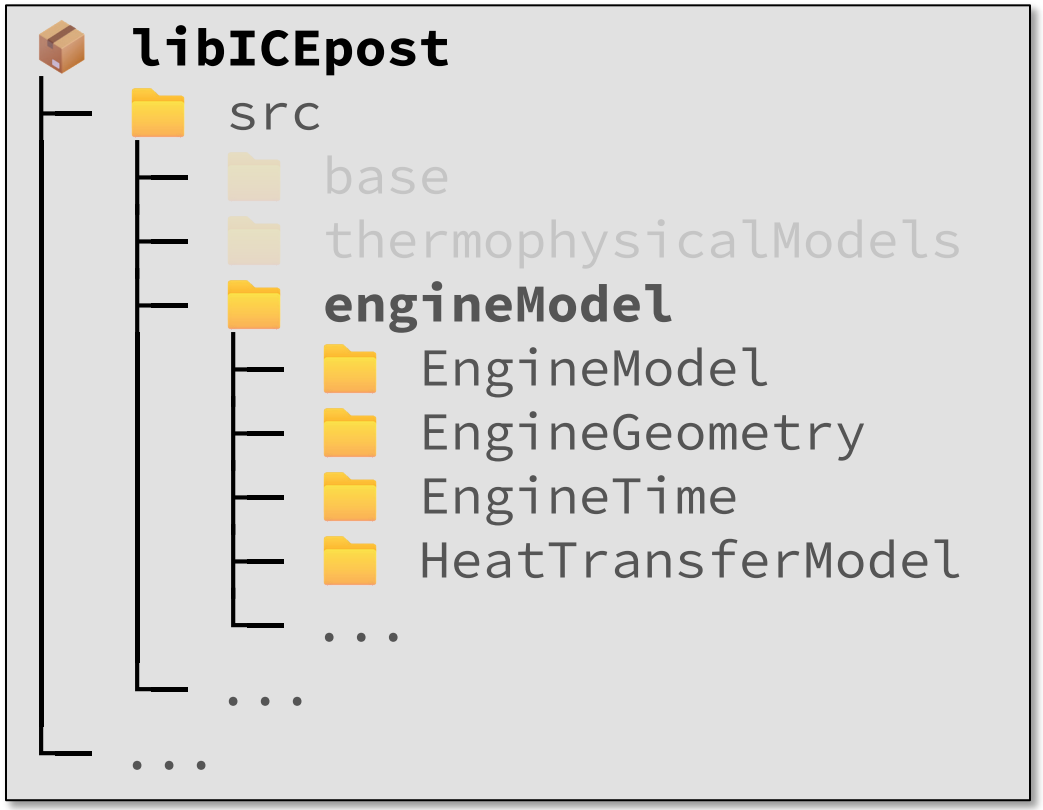
  - ➢ **thermoModels** – chemical and thermodynamic modeling of complex systems:
    - Thermodynamic properties of mixtures (mixing rules)
    - Combustion models (2-zone model, etc.)
    - Computation of exhaust-gas composition
    - Etc…



libICEpost.src.engineModel

- Classes for modeling of **internal combustion engines** (ICE)
- **Processing results** of measurements/simulations and extrapolate additional information on the **development of the combustion process**



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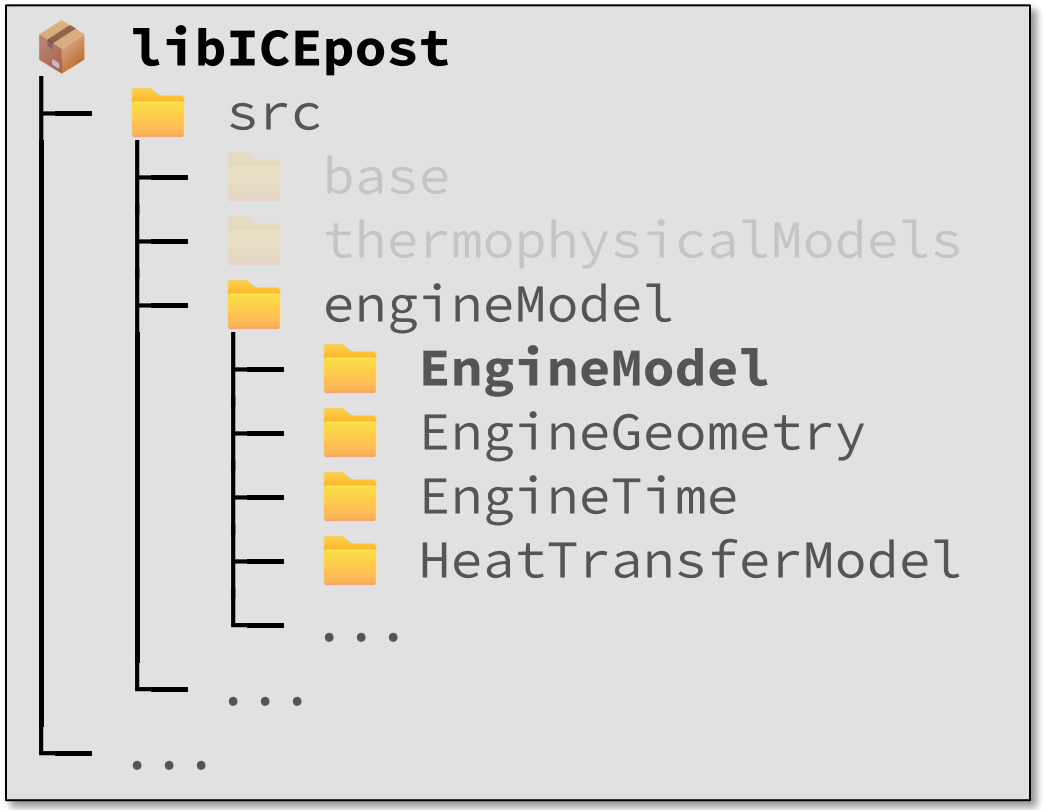
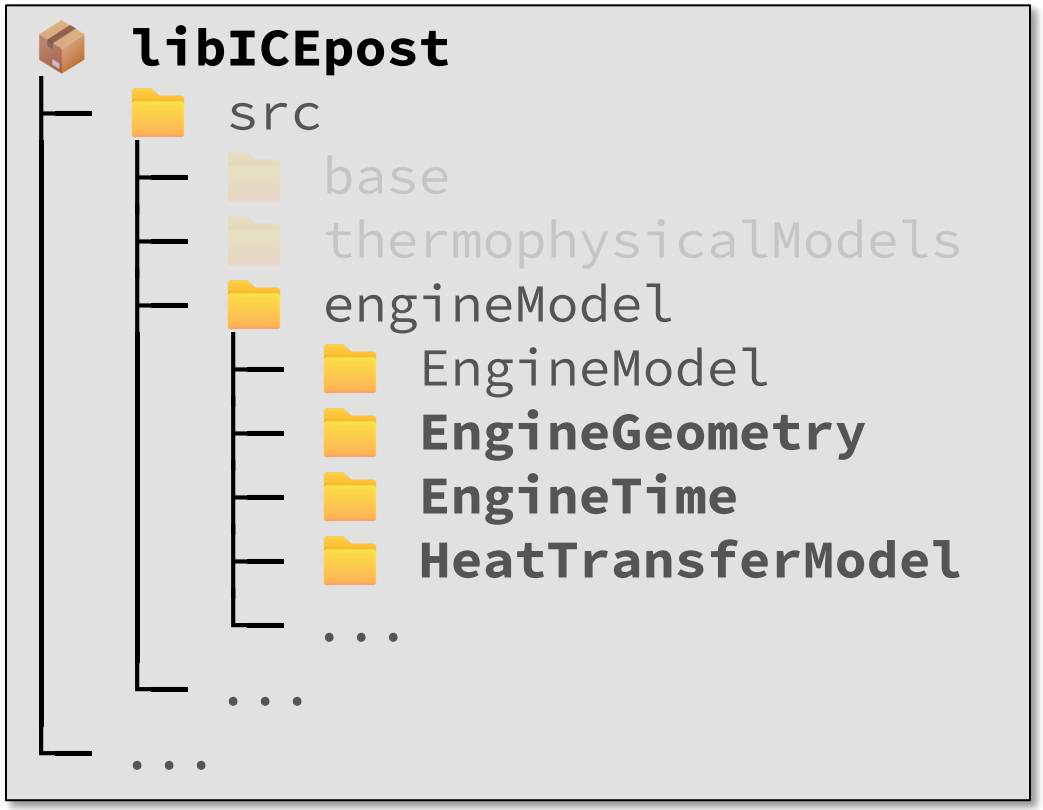


libICEpost.src.engineModel

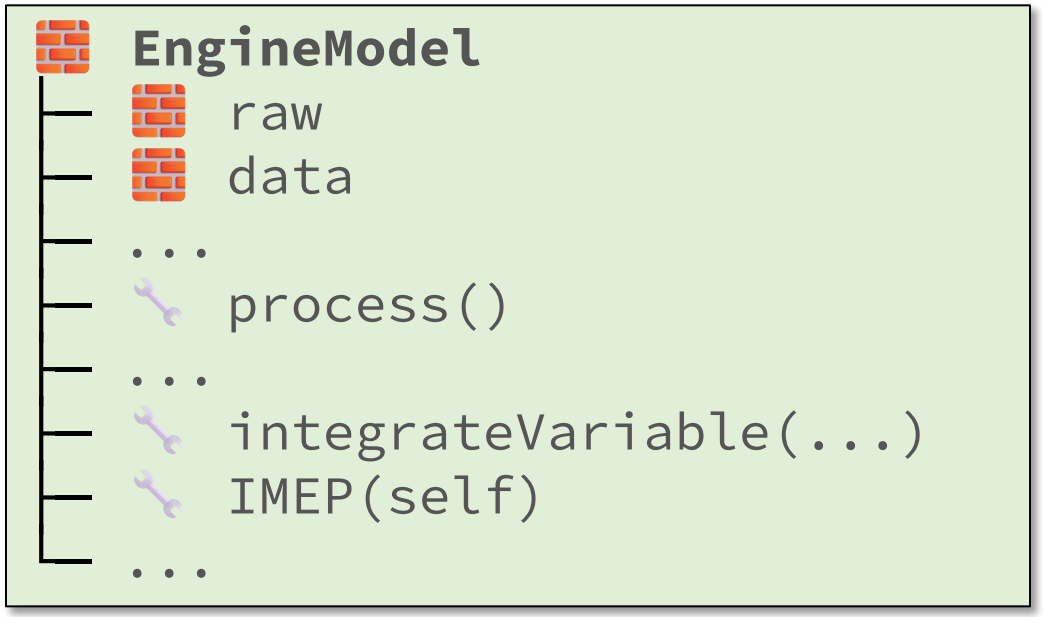
- Classes for modeling of **internal combustion engines** (ICE)
- **Processing results** of measurements/simulations and extrapolate additional information on the **development of the combustion process**

- **Main subpackages**:
  - `EngineModel` – defines the classes for **modeling of an engine configuration**, coupling all the sub-models
  - Multiple **sub-models** for handling specific aspects that may vary among different engine configurations, like:
    - `EngineTime`: handles the temporal evolution
    - `EngineGeometry`: geometrical features of the engine
    - `HeatTransferModel`: computes heat-transfer at walls



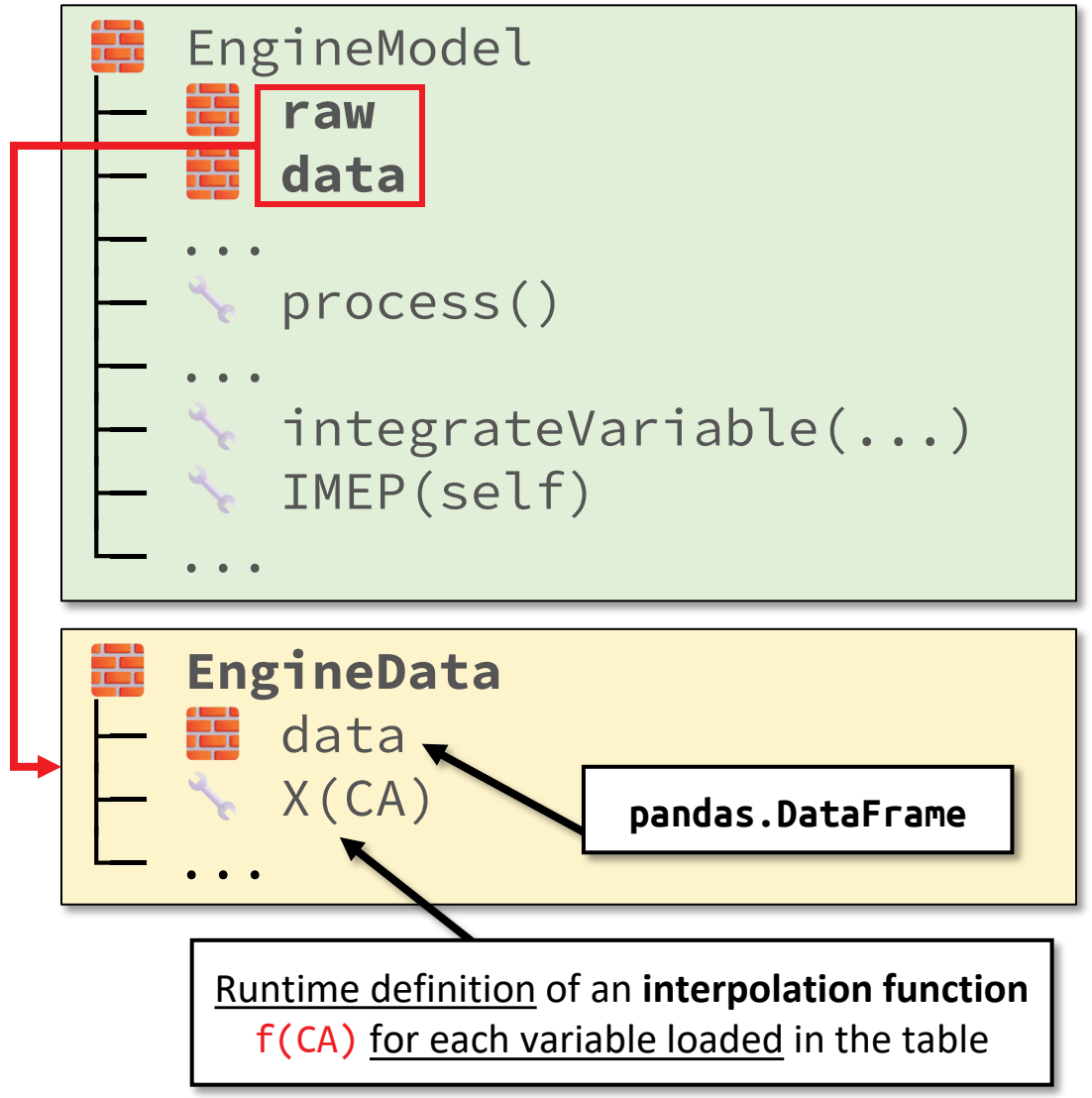
EngineModel class

- **Base class** for modeling ICE, implementing the **generic features** and coupling all the sub-models



EngineModel class

- **Base class** for modeling ICE, implementing the **generic features** and coupling all the sub-models
- **Structure of an `object` of this `class`:**
  - **Two data-structures** which contain the original (`raw`) and processed (`data`) data. They are instances of the `EngineData` class, a wrapper of a `pandas.DataFrame`



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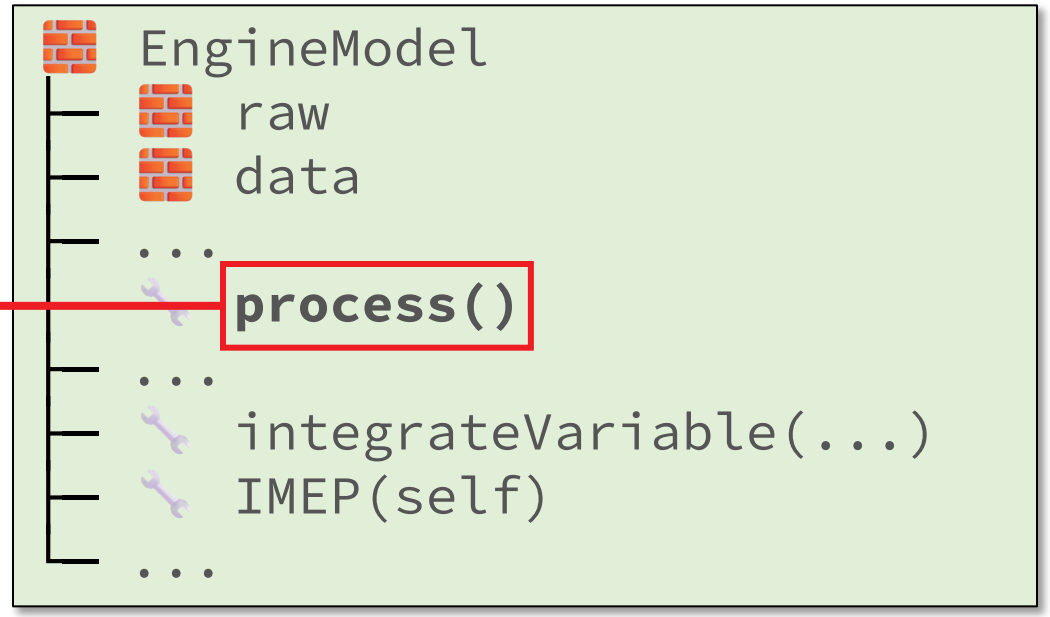


libICEpost\src\engineModel\EngineModel\EngineModel.py

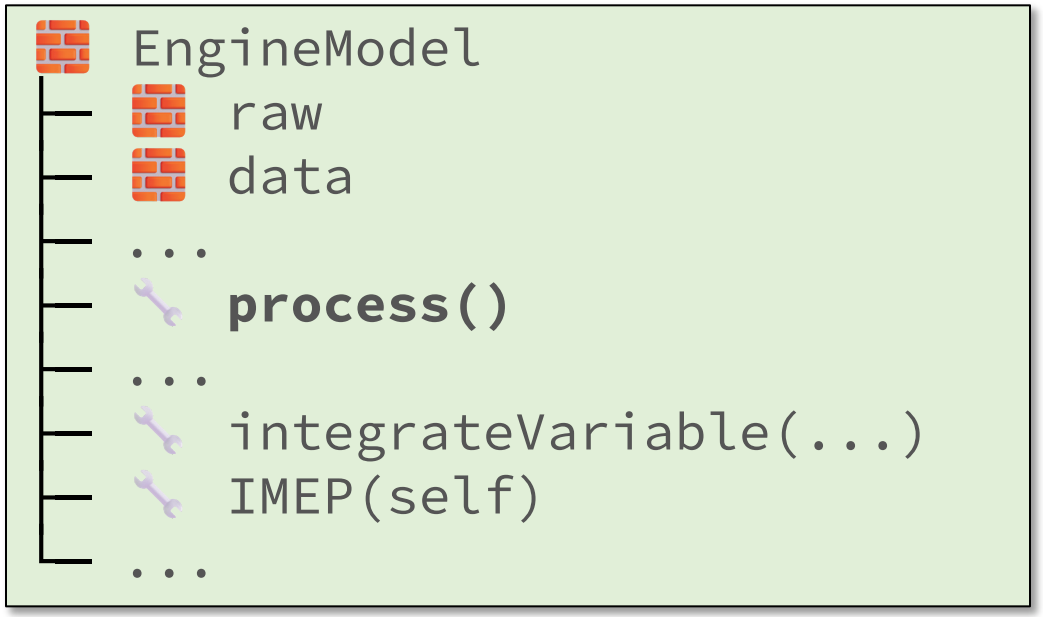
```python
def process(self):
    self._process__pre__() #Create fields

    #Process cylinder data - Main time loop
    for t in self.time(self.data["CA"]):
        self._update()

    #Final updates (heat transfer, cumulatives, etc...)
    self._process__post__()
```

EngineModel class

- **Base class** for modeling ICE, implementing the **generic features** and coupling all the sub-models
- **Structure of an `object` of this `class`:**
  - **Two data-structures** which contain the original (`raw`) and processed (`data`) data. They are instances of the `EngineData` class, a wrapper of a `pandas.DataFrame`
  - **`process()`** – The **main method** which processes the data and estimates the thermodynamic evolution of the system. Computes the **energy and mass balance** at the cylinder to estimate the apparent heat release rate (AHRR) and the rate of heat lease (ROHR) through the modelled wall heat flux ($\dot{Q}_{walls}$)



$$AHRR = \frac{dU_s}{d\theta} - \frac{dm_f}{d\theta} h_s + p\frac{dV}{d\theta}$$

Energy balance

$$ROHR = AHRR - \dot{Q}_{walls}$$

EngineModel class

- **Base class** for modeling ICE, implementing the **generic features** and coupling all the sub-models
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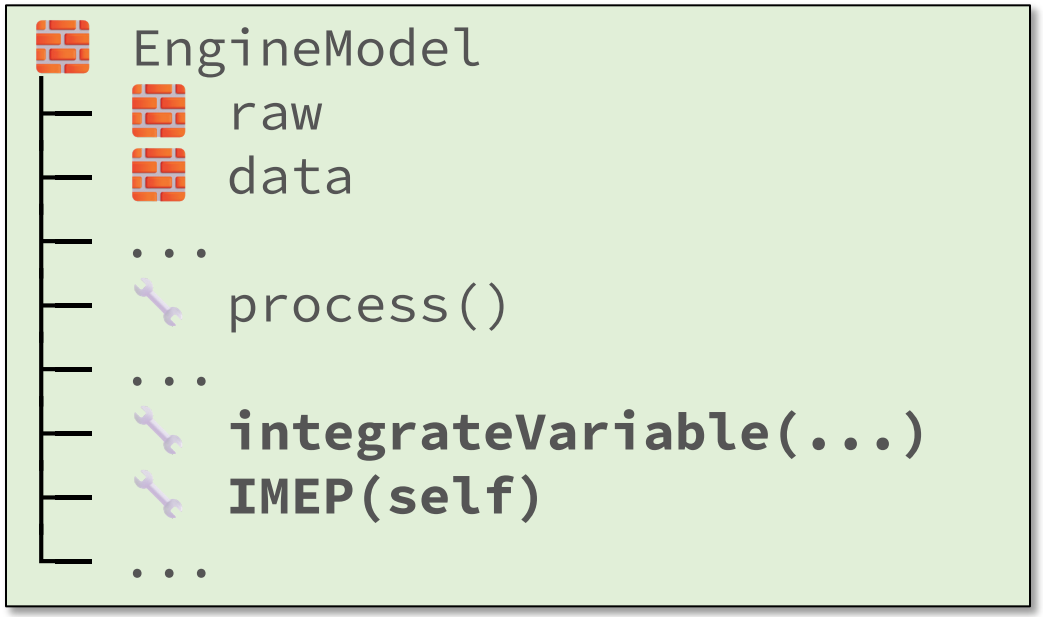
  - **Auxiliary methods** to extrapolate additional information from the processed data (integrating quantities, cumulative functions, work, etc.)



EngineModel class

- **Base class** for modeling ICE, implementing the **generic features** and coupling all the sub-models
- **Structure of an `object` of this `class`:**
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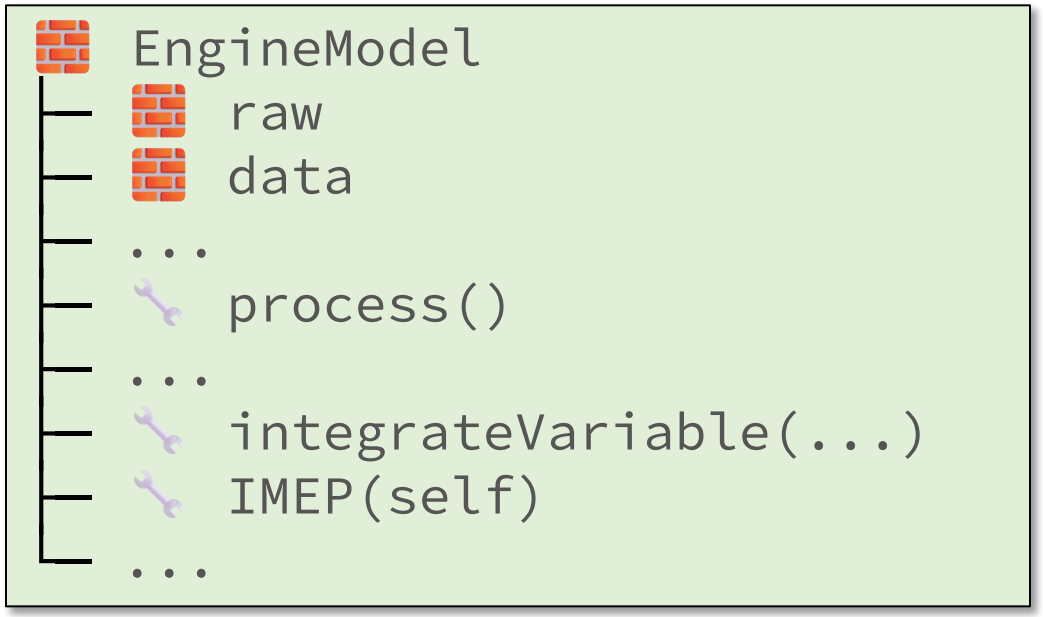
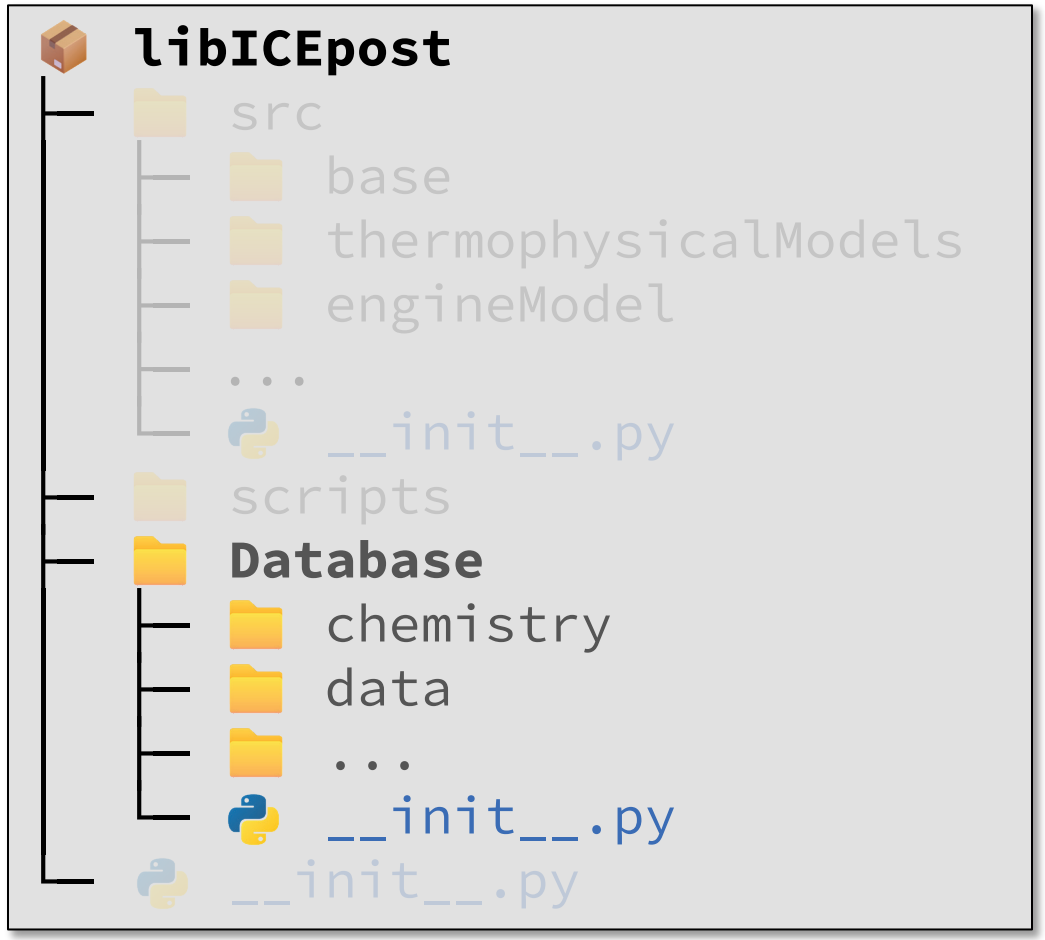
  - **Auxiliary methods** to extrapolate additional information from the processed data (integrating quantities, cumulative functions, work, etc.)
- References can be found in the `docs/` folder



libICEpost.Database

- A built-in database with useful data (periodic table, molecules, fuels, thermophysical properties, etc.)
- Contains the **variable database**: a container with a folder-like structure, which is dynamically populated loading the library sub-packages
- It accepts both dot (`.`) and key (`[str]`) access



libICEpost\Database__init__.py

```
1 from ._DatabaseClass import _DatabaseClass
2
3 database = _DatabaseClass("database")
```

Master folder "database"

libICEpost\Database\chemistry\constants.py

```
1 from libICEpost.Database import database
2
3 database.chemistry.addFolder("constants")
4
5 #Universal gas constant
6 database.chemistry.constants.Rgas = 8.314462*1e3 # [J/(kg K)]
```

Adding **named branches** (`_DatabaseClass` instances)

Populating the folders

libICEpost.Database

- A built-in database with useful data (periodic table, molecules, fuels, thermophysical properties, etc.)
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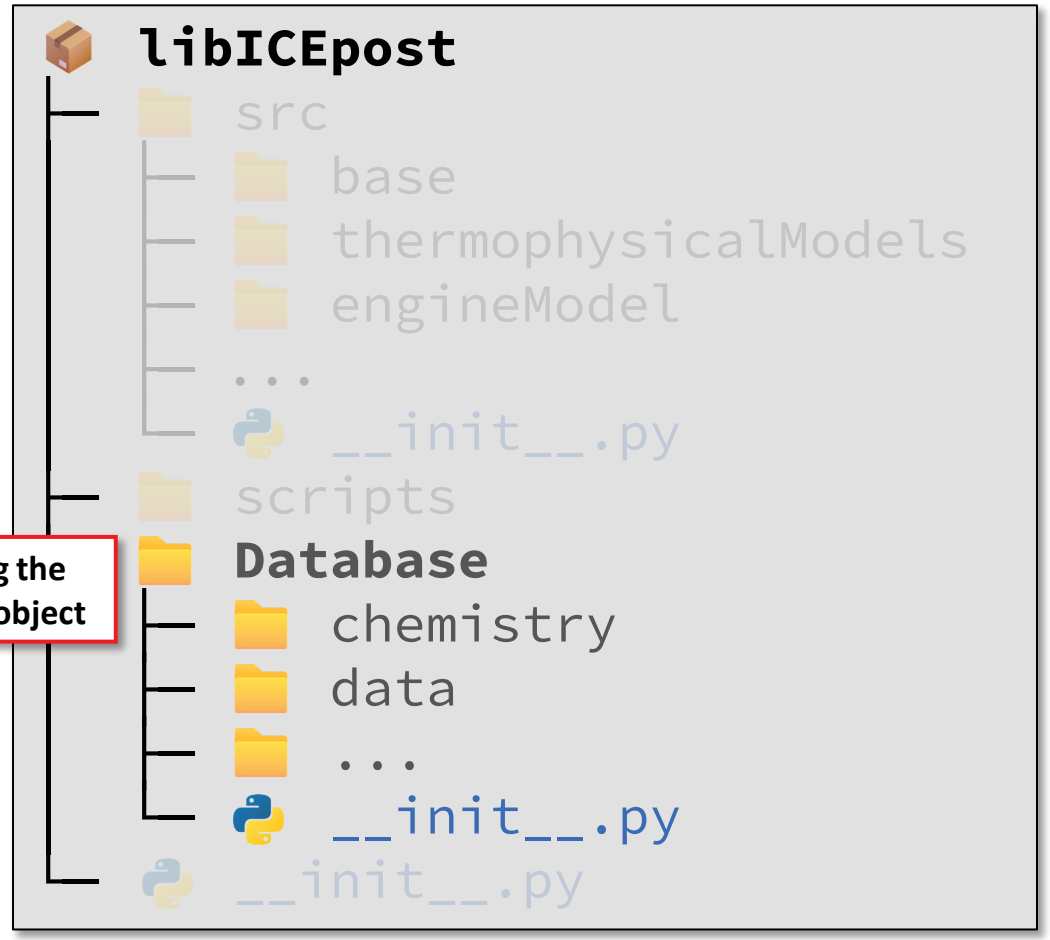
- It accepts both dot (`.`) and key (`[str]`) access

Loading mixtures in the database

Importing the database object

```
user@localhost: ~

>>> from libICEpost.Database.chemistry.specie.Mixtures import database
```



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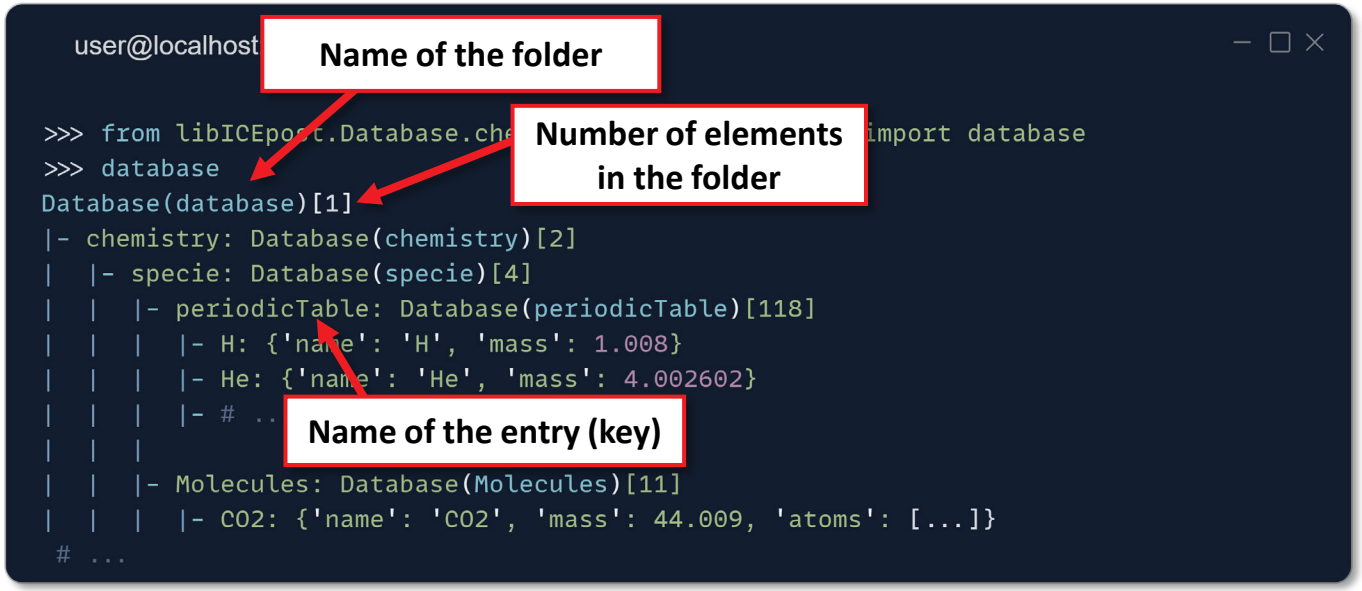

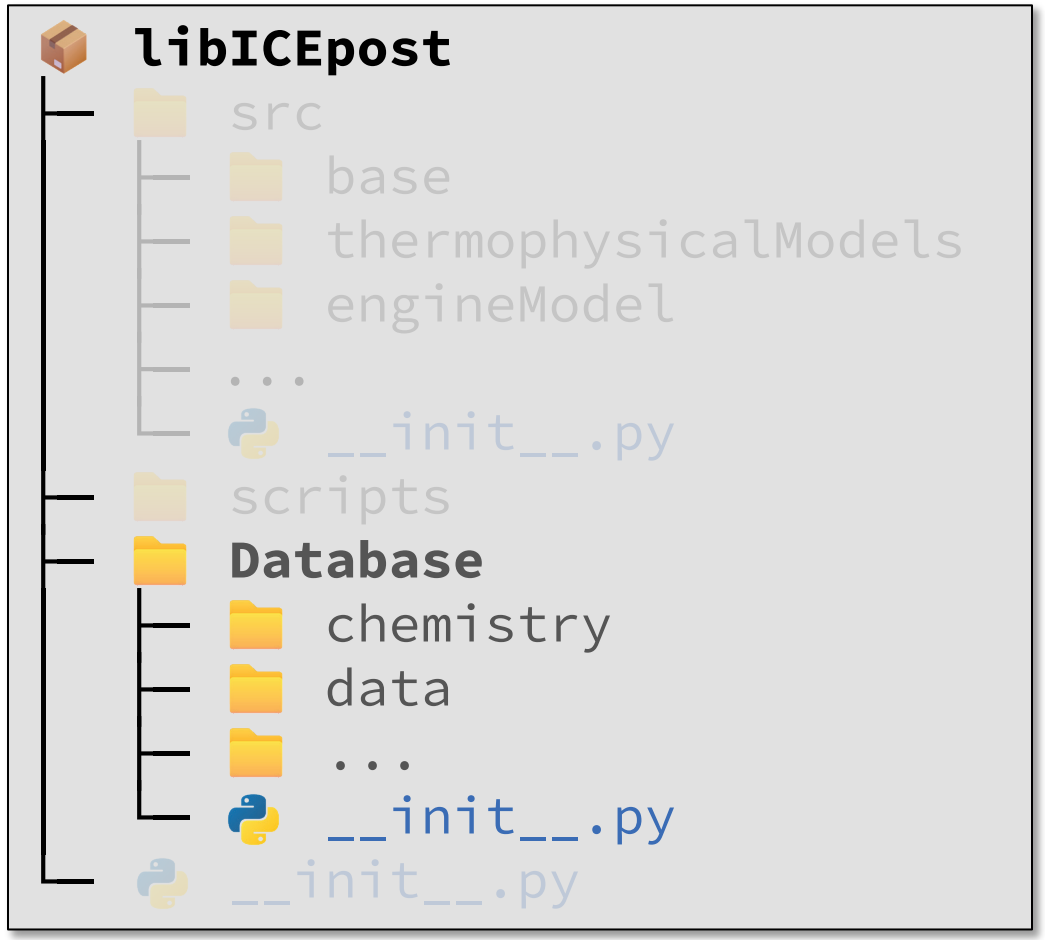

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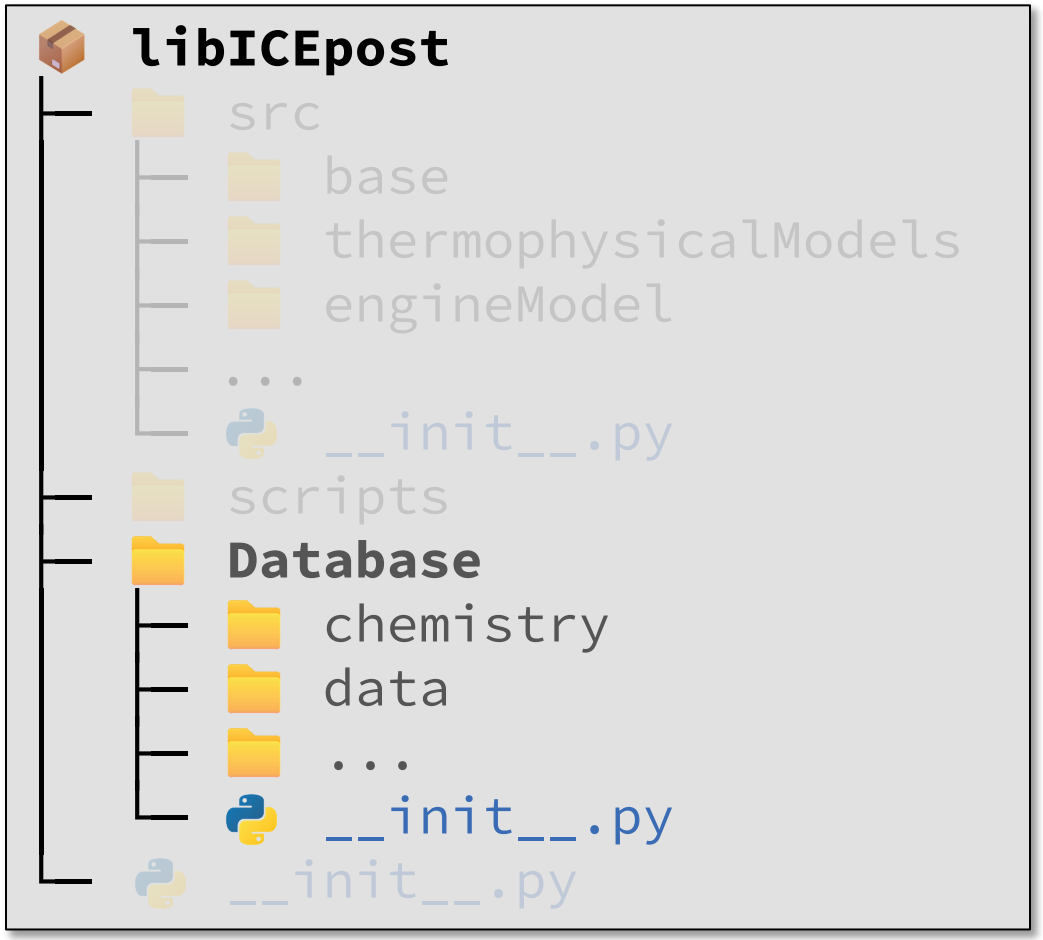


libICEpost\src\thermophysicalModels\specie\thermo\Thermo\janaf7.py

```
1 from libICEpost.Database import database
2 from libICEpost.Database.chemistry import constants
3 Tstd = database.chemistry.constants.Tstd
4 ...
```

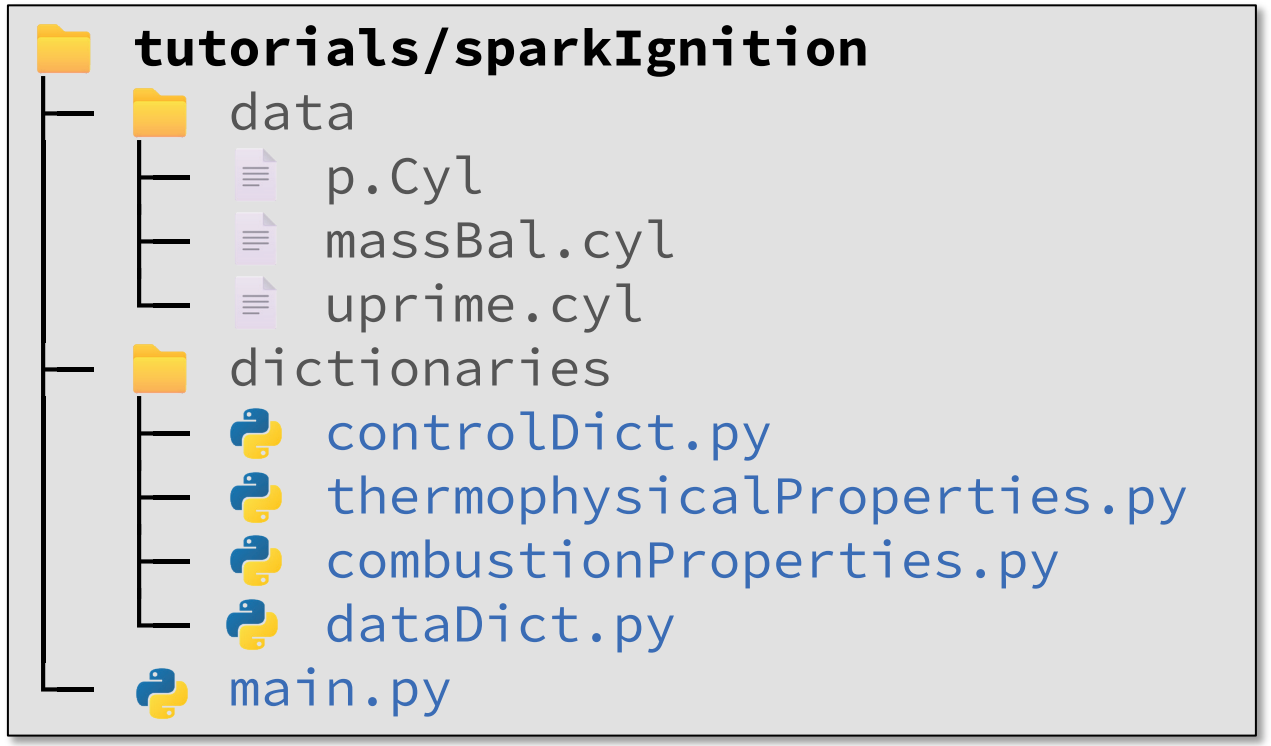
Loading the **database** instance

Loading the **sub-pachage**, which populates **database.chemistry.constants**

Accessing the variable

Example – CFD simulation of spark-ignition engine

- **Tutorial case**: post-process the results of a CFD simulation of a spark-ignition engine to extrapolate the rate of heat release profile.
- The tutorial can be found in the **GitHub repository** at `tutorials/sparkIgnition/`



Setup files

- **Tutorial case**: post-process the results of a CFD simulation of a spark-ignition engine to extrapolate the rate of heat release profile.
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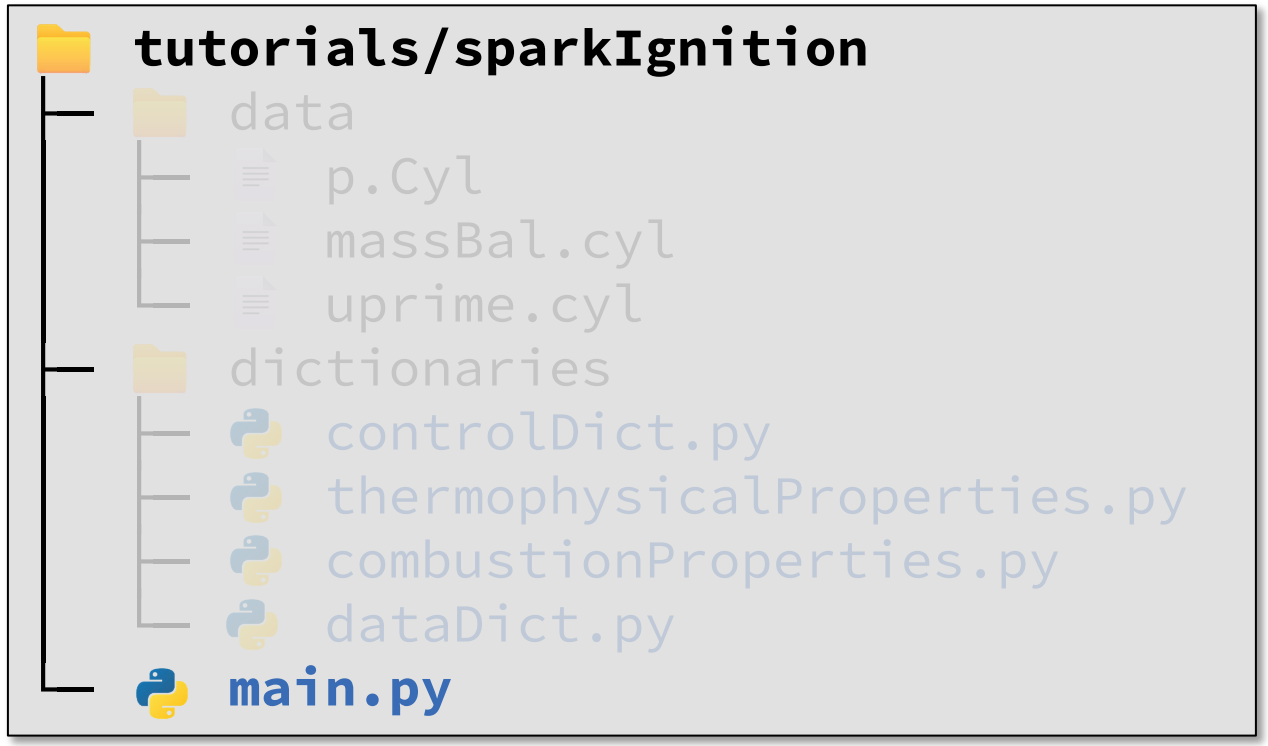
- **Content of the tutorial:**
  - **`main.py`** – The python script to be executed



Setup files

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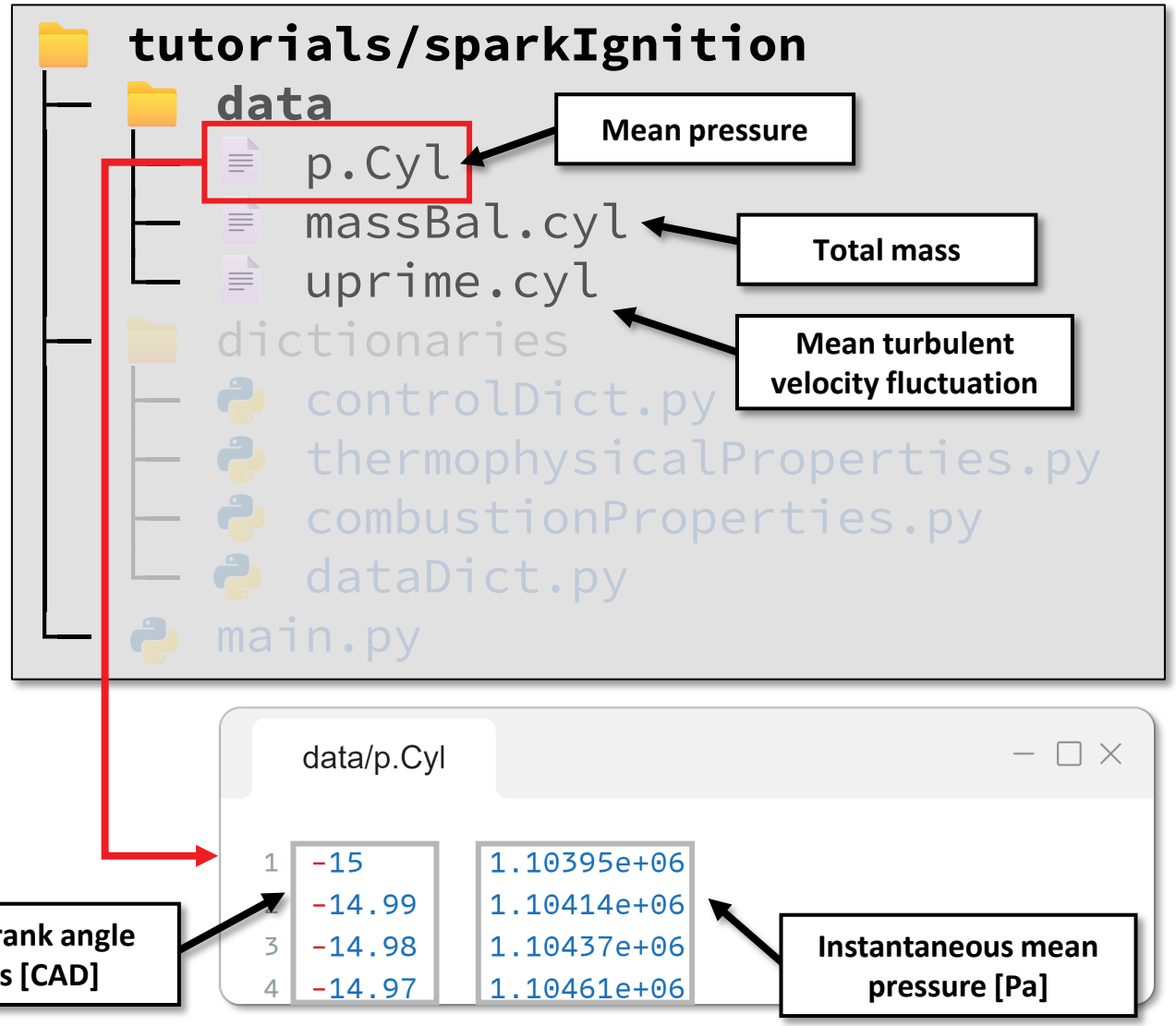
  - **`data`** – Contains **results of the CFD simulations**, i.e., in-cylinder traces of integral or average quantities



Setup files

- **Tutorial case**: post-process the results of a CFD simulation of a spark-ignition engine to extrapolate the rate of heat release profile.
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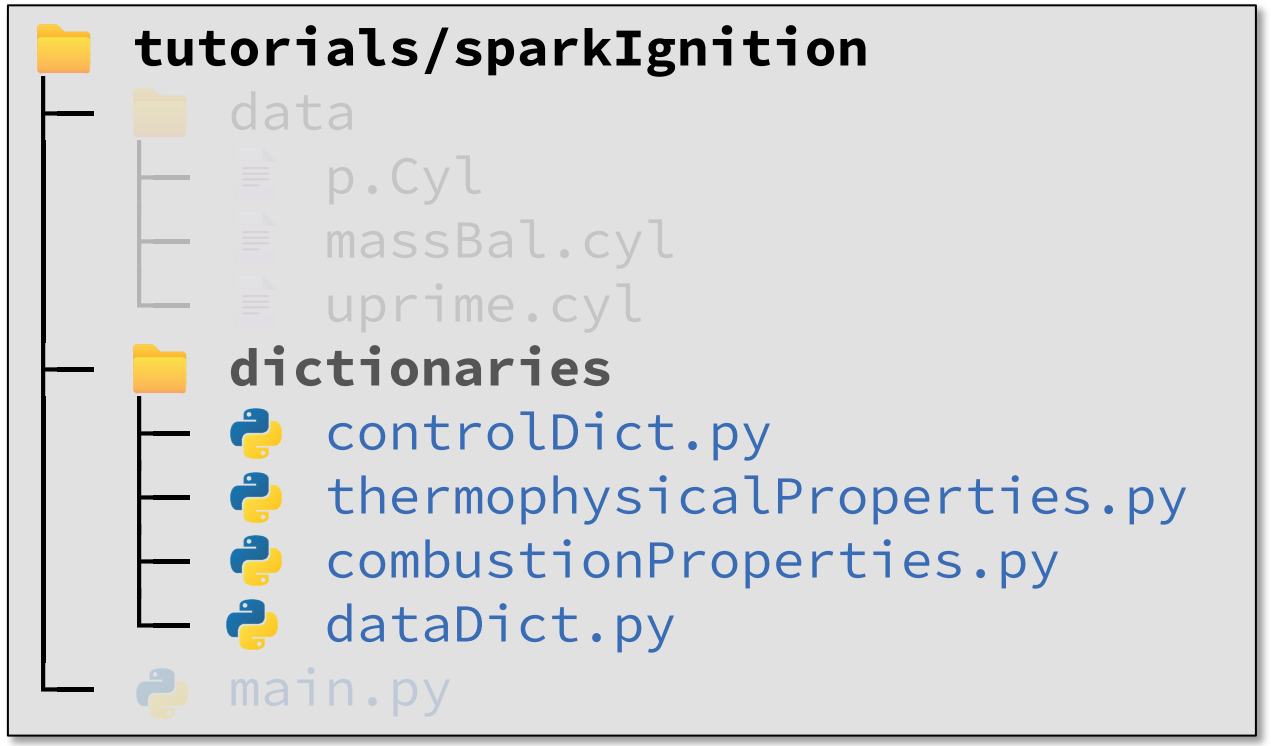
- **Content of the tutorial:**
  - `main.py` – The python script to be executed
  - `data` – Contains **results of the CFD simulations**, i.e., in-cylinder traces of integral or average quantities
  - `dictionaries` – Contains all the **dictionaries** that are used to construct the engine model



Setup files – `main.py`

Importing **`EngineModel`** and **`Dictionary`** from **`libICEpost`**

sparkIgnitionExample/main.py

```python
# -*- coding: utf-8 -*-
"""
Testing solver for post-processing of CFD results from spark-ignition simulations
"""

#Importing
import os
from libICEpost.src.engineModel.EngineModel.EngineModel import EngineModel
from libICEpost.src.base.dataStructures.Dictionary import Dictionary

#Getting the current path (needed when running in debug mode)
thisPath, _ = os.path.split(__file__)
print(f"thisPath = {thisPath}")
os.chdir(thisPath)  #Move here if in debug

# Load the constrol dictionary
controlDict = Dictionary.fromFile("./dictionaries/controlDict.py")

# Lookup engine model type and its dictionary
engineModelType:str = controlDict.lookup("engineModelType")
engineModelDict:Dictionary = controlDict.lookup(engineModelType + "Dict")

#Construct from run-time selector
model:EngineModel = EngineModel.selector(engineModelType, engineModelDict)

#Process the data in the engine model
model.process()

############################################################
# Combined plot of pressure trace and rate of heat release #
############################################################
#Importing matplotlib and pyplot
from matplotlib import pyplot as plt

```

Setup files – `main.py`

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model.process()

############################################################
# Combined plot of pressure trace and rate of heat release #
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#Importing matplotlib and pyplot
from matplotlib import pyplot as plt

```

Importing the **configuration of the engine model** from `controlDictionary.py` file into a **`Dictionary`** entry with the `fromFile` `classmethod`

Setup files – `main.py`

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model.process()

############################################################
# Combined plot of pressure trace and rate of heat release #
############################################################
#Importing matplotlib and pyplot
from matplotlib import pyplot as plt

```

Lookup the `EngineModel` to use and its construction dictionary and then construct it through the **`selector`** `classmethod`

Setup files – `main.py`

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# -*- coding: utf-8 -*-
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############################################################
# Combined plot of pressure trace and rate of heat release #
############################################################
#Importing matplotlib and pyplot
from matplotlib import pyplot as plt

```

Process the data loaded in the engine model

Setup files – `main.py`

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"""
Testing solver for post-processing of CFD results from spark-ignition simulations
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#Importing
import os
from libICEpost.src.engineModel.EngineModel.EngineModel import EngineModel
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# Lookup engine model type and its dictionary
engineModelType:str = controlDict.lookup("engineModelType")
engineModelDict:Dictionary = controlDict.lookup(engineModelType + "Dict")

#Construct from run-time selector
model:EngineModel = EngineModel.selector(engineModelType, engineModelDict)

#Process the data in the engine model
model.process()

############################################################
# Combined plot of pressure trace and rate of heat release #
############################################################
#Importing matplotlib and pyplot
from matplotlib import pyplot as plt

```

Plotting results

Setup files – controlDict.py

- This control dictionary contains the specific engine model to use and the construction dictionary of the corresponding class.

sparkIgnition\dictionaries\controlDict.py

```
#The type of engine model
engineModelType = "SparkIgnitionEngine"

#Properties of the specific EngineModel sub-class
SparkIgnitionEngineDict = \
{
    #The sub-class handling time
    "EngineTime": "SparkIgnitionTime",
    "SparkIgnitionTimeDict": \
    {
        "IVC": -130, #[CAD]
        "EVO": 100,  #[CAD]
        "speed": 800,#[rpm]
        "SA": -14.2  #[CAD]
    },

    #The sub-class handling the engine geometrical parameters
    "EngineGeometry": "ConRodGeometry",
    "ConRodGeometryDict": \
    {
        "bore": 86e-3,       #[m]
        "stroke": 86e-3,     #[m]
        "conRodLen": 148e-3, #[m]
        "CR":8.7,            #[-]
    },
```

Setup files – controlDict.py

- This control dictionary contains the specific engine model to use and the construction dictionary of the corresponding class.

- The **construction dictionary** must contain:
  - TypeName and construction dictionary (in the form <TypeName>Dict) for **EngineTime** and **EngineGeometry sub-models**

sparkIgnition\dictionaries\controlDict.py

```
#The type of engine model
engineModelType = "SparkIgnitionEngine"

#Properties of the specific EngineModel sub-class
SparkIgnitionEngineDict = \
{
    #The sub-class handling time
    "EngineTime": "SparkIgnitionTime",
    "SparkIgnitionTimeDict": \
    {
        "IVC": -130, #[CAD]
        "EVO": 100,  #[CAD]
        "speed": 800,#[rpm]
        "SA": -14.2  #[CAD]
    },

    #The sub-class handling the engine geometrical parameters
    "EngineGeometry": "ConRodGeometry",
    "ConRodGeometryDict": \
    {
        "bore": 86e-3,       #[m]
        "stroke": 86e-3,     #[m]
        "conRodLen": 148e-3, #[m]
        "CR":8.7,            #[-]
    },
```

Setup files – `controlDict.py`

- This control dictionary contains the specific engine model to use and the construction dictionary of the corresponding class.
- The **construction dictionary** must contain:
  - `TypeName` and construction dictionary (in the form `<TypeName>Dict`) for **`EngineTime`** and **`EngineGeometry`** sub-models
  - Two dictionaries containing the **thermophysical** and **combustion properties** of mixtures

sparkIgnition\dictionaries\controlDict.py

```
28
29      #Dictionary for thermophysical properties
30      "thermophysicalProperties":\
31          Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
32
33      #Dictionary for combustion properties
34      "combustionProperties":\
35          Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
36
37      #Dictionary for data loading
38      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py"),
39
40      #Dictionary for specific sub-models
41      "submodels":\
42          {
43              #Heat transfer model
44              "HeatTransferModelType":"Woschni",
45              "WoschniDict":{} #Default coefficients
46          }
47  }
```

Setup files – controlDict.py

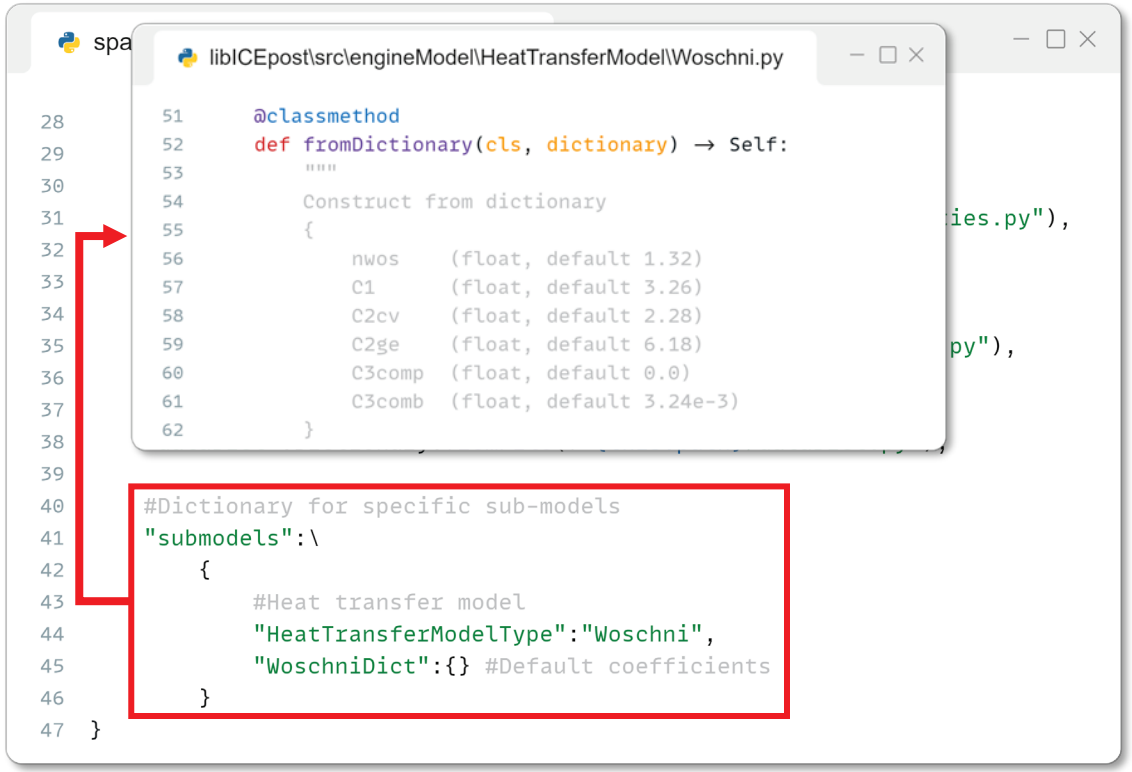
- This control dictionary contains the specific engine model to use and the construction dictionary of the corresponding class.
- The **construction dictionary** must contain:
  - TypeName and construction dictionary (in the form <TypeName>Dict) for **EngineTime** and **EngineGeometry sub-models**
  - Two dictionaries containing the **thermophysical** and **combustion properties** of mixtures
  - A dictionary containing the information for **loading input data** and **pre-processing** (filtering, scaling, etc.)

sparkIgnition\dictionaries\controlDict.py

```
28
29      #Dictionary for thermophysical properties
30      "thermophysicalProperties":\
31          Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
32
33      #Dictionary for combustion properties
34      "combustionProperties":\
35          Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
36
37      #Dictionary for data loading
38      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py"),
39
40      #Dictionary for specific sub-models
41      "submodels":\
42          {
43              #Heat transfer model
44              "HeatTransferModelType":"Woschni",
45              "WoschniDict":{} #Default coefficients
46          }
47  }
```

Setup files – controlDict.py

- This control dictionary contains the specific engine model to use and the construction dictionary of the corresponding class.
- The **construction dictionary** must contain:
  - TypeName and construction dictionary (in the form <TypeName>Dict) for **EngineTime** and **EngineGeometry sub-models**
  - Two dictionaries containing the **thermophysical** and **combustion properties** of mixtures
  - A dictionary containing the information for **loading input data** and **pre-processing** (filtering, scaling, etc.)
  - A dictionary containing the specific information of other sub-models (e.g. heat transfer)



Setup files – thermophysicalProperties

- **thermophysicalProperties**:
  - **thermoType** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)

sparkIgnitionExample/controlDict.py

```
27  #Dictionary for thermophysical properties
28  "thermophysicalProperties":\
29  Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31  #Dictionary for combustion properties
32  "combustionProperties":\
33  Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35  #Dictionary for data loading
36  "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/thermophysicalProperties.py

```
1  #Classes to use for construction of the thermodynamic type
2  thermoType = \
3      {
4          #The equation of state to use
5          "EquationOfState":"PerfectGas", #Perfect gas assumption
6
7          #The thermodynamic properties for the mixture
8          "Thermo":"janaf7",  # 7-coefficients NASA (janaf) polynomials
9      }
10
11 #Dictionaries for class-specific entries
12 PerfectGasDict = {}
13 janaf7Dict = {}
```

Setup files – thermophysicalProperties

- **thermophysicalProperties**:
  - **thermoType** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/thermophysicalProperties.py

```
1  #Classes to use for construction of the thermodynamic type
2  thermoType = \
3      {
4          #The equation of state to use
5          "EquationOfState":"PerfectGas", #Perfect gas assumption
6
7          #The thermodynamic properties for the mixture
8          "Thermo":"janaf7",  # 7-coefficients NASA (janaf) polynomials
9      }
10
11 #Dictionaries for class-specific entries
12 PerfectGasDict = {}
13 janaf7Dict = {}
```

Setup files – combustionProperties

- **thermophysicalProperties**:
  - **thermoType** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models

- **combustionProperties**:

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/combustionProperties.py

Loading properties from database

```
1  #Loading mixtures and molecules from database
2  from libICEpost.Database.chemistry.specie.Mixtures import Mixtures, Mixture
3  from libICEpost.Database.chemistry.specie.Molecules import Fuels
4  air = Mixtures.dryAir   #Standard air composition
5
6  #Dictionary for computation of initial mixture composition in each region
7  initialMixture = \
8  {
9      #In-cylinder region
10     "cylinder":
11         {
12         #Information for the premixed fuel
13         "premixedFuel": \
14             {
15                 #The mixture of the fuel (pure iso-octane)
```

Setup files – combustionProperties

- **thermophysicalProperties**:
  - **thermoType** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models

- **combustionProperties**:
  - **air** – The specific Mixture to use for air (oxidizer)

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/combustionProperties.py

Using the entry from database

```
1  #Loading mixtures a                    e
2  from libICEpost.Database.chemistry.specie.Mixtures import Mixtures, Mixture
3  from libICEpost.Database.chemistry.specie.Molecules import Fuels
4  air = Mixtures.dryAir    #Standard air composition
5
6  #Dictionary for computation of initial mixture composition in each region
7  initialMixture = \
8  {
9      #In-cylinder region
10     "cylinder":
11         {
12         #Information for the premixed fuel
13         "premixedFuel": \
14             {
15                 #The mixture of the fuel (pure iso-octane)
```

Setup files – combustionProperties

- **thermophysicalProperties**:
  - **thermoType** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models

- **combustionProperties**:
  - **air** – The specific Mixture to use for air (oxidizer)
  - **initialMixture** – A dictionary for **initialization of the mixture** inside o each thermodynamic region

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/combustionProperties.py

```
6  #Dictionary for computation of initial mixture composition in each region
7  initialMixture = \
8  {
9      #In-cylinder region
10     "cylinder":
11         {
12         #Information for the premixed fuel
13         "premixedFuel": \
14             {
15                 #The mixture of the fuel (pure iso-octane)
16                 "mixture": Mixture([Fuels.IC8H18], [1.0]),
17
18                 #The equivalence ratio of the mixture
19                 "phi":1.0,
20             },
21         }
```

Using the entry from database

Setup files – combustionProperties

- **thermophysicalProperties**:
  - **thermoType** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models
- **combustionProperties**:
  - **air** – The specific Mixture to use for air (oxidizer)
  - **initialMixture** – A dictionary for **initialization of the mixture** inside o each thermodynamic region
  - The model to compute the exhaust gas composition

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/combustionProperties.py

```
22  }
23
24  # The model to account for exhaust-gas recirculation
25  # on in-cylinder mixture composition
26  EgrModel = "StoichiometricMixtureEGR" #EGR composition computed at lambda = 1
27
28  StoichiometricMixtureEGRDict = \
29  {
30      "air":Mixtures.dryAir,
31      "fuel":Mixture([Fuels.IC8H18], [1.0]),
32      "egr":0.115,
33      "combustionEfficiency":0.9
34  }
35
36  # Giving separately the mass-fractions of externally
```

Setup files – combustionProperties

- **thermophysicalProperties**:
  - **thermoType** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models

- **combustionProperties**:
  - **air** – The specific Mixture to use for air (oxidizer)
  - **initialMixture** – A dictionary for **initialization of the mixture** inside o each thermodynamic region
  - The model to compute the exhaust gas composition
  - The **combustion model** to use to estimate the instantaneous mixture composition

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/combustionProperties.py

```
38  ExternalInterEGRDict = \
39  {
40      "externalEGR":0.0,
41      "internalEGR":0.0,
42      "combustionEfficiency":0.9
43  }
44
45  #The combustion model used (spark-ignition)
46  CombustionModel = "PremixedCombustion" #Premixed combustion
47  PremixedCombustionDict = \
48  {
49      #The reaction model used to compute the mixture composition
50      "reactionModel":"Stoichiometry", # Stoichiometric-reaction
51                                       # combustion products
52                                       # [Reactants] → [Products]
53  }
```

Setup files – dataDict

- **thermophysicalProperties**:
  - **thermoType** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models
- **combustionProperties**:
  - **air** – The specific Mixture to use for air (oxidizer)
  - **initialMixture** – A dictionary for **initialization of the mixture** inside o each thermodynamic region
  - The model to compute the exhaust gas composition
  - The **combustion model** to use to estimate the instantaneous mixture composition
- **dataDict**:
  - **dataPath** – The master path for input/output of data

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/dataDict.py

```
1  #Global path where data are stored
2  dataPath = f"{this.path}/../data"
3
4  #The fields to load for each region
5  data = \
6  {
7      #Data for the cylinder region
8      "cylinder":\
9      {
10         #Pressure (mandatory)
11         "p":\
12         {
13             #The format of the data to load
14             "format":"file",    #Retreive from file
15
```

Setup files – `dataDict`

- **`thermophysicalProperties`**:
  - **`thermoType`** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models
- **`combustionProperties`**:
  - **`air`** – The specific `Mixture` to use for air (oxidizer)
  - **`initialMixture`** – A dictionary for **initialization of the mixture** inside o each thermodynamic region
  - The model to compute the exhaust gas composition
  - The **combustion model** to use to estimate the instantaneous mixture composition
- **`dataDict`**:
  - **`dataPath`** – The master path for input/output of data
  - **`data`** – dictionary with the fields to be loaded for each thermodynamic region

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/dataDict.py

```
1  #Global path where data are stored
2  dataPath = f"{this.path}/../data"
3
4  #The fields to load for each region
5  data = \
6  {
7      #Data for the cylinder region
8      "cylinder":\
9      {
10         #Pressure (mandatory)
11         "p":\
12         {
13             #The format of the data to load
               "format":"file",    #Retreive from file
```

Region name

Field name

Setup files – `dataDict`

- **`thermophysicalProperties`**:
  - **`thermoType`** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models
- **`combustionProperties`**:
  - **`air`** – The specific `Mixture` to use for air (oxidizer)
  - **`initialMixture`** – A dictionary for **initialization of the mixture** inside o each thermodynamic region
  - The model to compute the exhaust gas composition
  - The **combustion model** to use to estimate the instantaneous mixture composition
- **`dataDict`**:
  - **`dataPath`** – The master path for input/output of data
  - **`data`** – dictionary with the fields to be loaded for each thermodynamic region

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/dataDict.py

```
11          "p":\
12          {
13              #The format of the data to load
14              "format":"file",    #Retreive from file
15
16              #The parameters to use
17              "data":
18              {
19                  #Name of the file
20                  "fileName":"p.Cyl",
21
22                  #Options to apply (scaling, shifting, etc.)
23                  "opts":{}
24              }
25          },
```

Format for loading the variable. Multiple formats available (see example file for more)

File name (relative to `dataPath`)

Setup files – `dataDict`

- **`thermophysicalProperties`**:
  - **`thermoType`** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models
- **`combustionProperties`**:
  - **`air`** – The specific `Mixture` to use for air (oxidizer)
  - **`initialMixture`** – A dictionary for **initialization of the mixture** inside o each thermodynamic region
  - The model to compute the exhaust gas composition
  - The **combustion model** to use to estimate the instantaneous mixture composition
- **`dataDict`**:
  - **`dataPath`** – The master path for input/output of data
  - **`data`** – dictionary with the fields to be loaded for each thermodynamic region
  - **`preProcessing`** – manipulation of data before processing (resampling, denoising, etc.)

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/dataDict.py

```
84
85  #Parameters for pre-processing of data
86  preProcessing = \
87  {
88      #Filter to apply on the data-set
89      "Filter":"Resample", # Resampling over uniform grid
90      "ResampleDict":\
91          {
92              "delta":1.0 #Delta-t [CA]
93          },
94
95      #User-defined filter through function/lambda such as:
96      #f(Iterable,Iterable) → tuple[Iterable,Iterable]
97      "UserDefinedFilterDict":\
98          {
99              "function": lambda x,y : (x,y) #Dummy no-filter function
```

Setup files – `dataDict`

- **`thermophysicalProperties`**:
  - **`thermoType`** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models
- **`combustionProperties`**:
  - **`air`** – The specific `Mixture` to use for air (oxidizer)
  - **`initialMixture`** – A dictionary for **initialization of the mixture** inside o each thermodynamic region
  - The model to compute the exhaust gas composition
  - The **combustion model** to use to estimate the instantaneous mixture composition
- **`dataDict`**:
  - **`dataPath`** – The master path for input/output of data
  - **`data`** – dictionary with the fields to be loaded for each thermodynamic region
  - **`preProcessing`** – manipulation of data before processing (resampling, denoising, etc.)

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/dataDict.py

```
84
85  #Parameters for pre-processing of data
86  preProcessing = \
87  {
88      #Filter to apply on the data-set
89      "Filter":"Resample", # Resampling over uniform grid
90      "ResampleDict":\
91          {
92              "delta":1.0 #Delta-t [CA]
93          },
94
95      #User-defined filter through fu
96      #f(Iterable,Iterable) → tuple[
97      "UserDefinedFilterDict":\
98          {
99              "function": lambda x,y
```

Resampling of data over uniform grid. **Optimal ΔT of 1 CAD** for accuracy and processing time

Setup files – `dataDict`

- `thermophysicalProperties`:
  - **`thermoType`** – how to construct the **thermodynamic model of mixtures**, namely the equation of state and the thermal properties (c_p, c_v, h_f, etc.)
  - Specific information required by the models
- `combustionProperties`:
  - **`air`** – The specific `Mixture` to use for air (oxidizer)
  - **`initialMixture`** – A dictionary for **initialization of the mixture** inside o each thermodynamic region
  - The model to compute the exhaust gas composition
  - The **combustion model** to use to estimate the instantaneous mixture composition
- **`dataDict`**:
  - **`dataPath`** – The master path for input/output of data
  - **`data`** – dictionary with the fields to be loaded for each thermodynamic region
  - **`preProcessing`** – manipulation of data before processing (resampling, denoising, etc.)
  - **`initialConditions`** – initial state of each region

sparkIgnitionExample/controlDict.py

```
27      #Dictionary for thermophysical properties
28      "thermophysicalProperties":\
29      Dictionary.fromFile(f"{this.path}/thermophysicalProperties.py"),
30
31      #Dictionary for combustion properties
32      "combustionProperties":\
33      Dictionary.fromFile(f"{this.path}/combustionProperties.py"),
34
35      #Dictionary for data loading
36      "dataDict":Dictionary.fromFile(f"{this.path}/dataDict.py")
37
```

sparkIgnitionExample/dataDict.py

```
107             "delta":1.0 #Delta-t over which resampling after filtering
108         }
109 }
110
111 #Initial conditions each thermodynamic region
112 initialConditions = \
113 {
114     #In-cylinder region (at closed-valves)
115     "cylinder": \
116     {
117         "pressure":"p",          #Interpolation from field 'p'
118         "mass":"m_CFD",          #Interpolation from field 'm_CFD'
119         "volume":"@geometry.V", #From the method self.geometry.V(CA)
120         "xb":0.0,                #Value
121     }
```

Plotting results

Generating the figure and axes: left axis for pressure trace and right for ROHR

sparkIgnitionExample/main.py

```
47      'figure.figsize':(6,12),
48      # 'figure.dpi':10
49  })
50
51  #Create figure and combined axes (pressure lefr, ROHR right)
52  fig, axP = plt.subplots(1,1, figsize=(6,8))
53  axRohr = axP.twinx()
54
55  #Processed data are stored in the entry 'model.data' of type EngineData.
56  #This is a wrapper around a pandas.DataFrame data-structure, which is
57  #the entry EngineModel.data. Hence we use the method DataFrame.plot, which
58  #is a convenient interface for plotting of the data inside the DataFrame instance
59
60  #Pressure
61  model.data.data.plot(\
62      x="CA", y="pBar",                          #x and y variables
63      c="k", ylabel="p [bar]", xlabel="[CAD]",   #Formatting
64      ax=axP,                                    #Axes
65      legend=False)                              #No legend
66
67  #Rate of heat release (ROHR)
68  model.data.data.plot(\
69      x="CA", y="ROHR",                          #x and y variables
70      c="k", ls="--", ylabel="ROHR [J/CA]",      #Formatting
71      ax=axRohr,                                 #Axes
72      legend=False)                              #No legend
73
74  #Adjust axes and limits
75  plt.tight_layout()
76  axP.set_xlim((-30,30))  #x axis
77  axP.set_ylim((-10,40))  #pressure
78  axRohr.set_ylim((0,100)) #ROHR
79
80  #Show the figure
81  plt.show()
```

Plotting results

sparkIgnitionExample/main.py

```
47      'figure.figsize':(6,12),
48      # 'figure.dpi':10
49  })
50
51  #Create figure and combined axes (pressure lefr, ROHR right)
52  fig, axP = plt.subplots(1,1, figsize=(6,8))
53  axRohr = axP.twinx()
54
55  #Processed data are stored in the entry 'model.data' of type Engin
56  #This is a wrapper around a pandas.DataFrame data-structure, which
57  #the entry EngineModel.data. Hence we use the method DataFrame.plot
58  #is a convenient interface for plotting of the data inside the Data
59
60  #Pressure
61  model.data.data.plot(\
62      x="CA", y="pBar",                          #x and y variables
63      c="k", ylabel="p [bar]", xlabel="[CAD]",   #Formatting
64      ax=axP,                                    #Axes
65      legend=False)                              #No legend
66
67  #Rate of heat release (ROHR)
68  model.data.data.plot(\
69      x="CA", y="ROHR",                          #x and y variables
70      c="k", ls="--", ylabel="ROHR [J/CA]",      #Formatting
71      ax=axRohr,                                 #Axes
72      legend=False)                              #No legend
73
74  #Adjust axes and limits
75  plt.tight_layout()
76  axP.set_xlim((-30,30))  #x axis
77  axP.set_ylim((-10,40))  #pressure
78  axRohr.set_ylim((0,100)) #ROHR
79
80  #Show the figure
81  plt.show()
```

Accessing the results at `model.data`, which is a `EngineData` instance. Then accessing the `data` entry, which is of type `pandas.DataFrame`, which has the convenient method **`plot`** for visualizing the stored data

Plotting results

Pressure trace on left axis

ROHR on right axis

sparkIgnitionExample/main.py

```
47      'figure.figsize':(6,12),
48      # 'figure.dpi':10
49  })
50
51  #Create figure and combined axes (pressure lefr, ROHR right)
52  fig, axP = plt.subplots(1,1, figsize=(6,8))
53  axRohr = axP.twinx()
54
55  #Processed data are stored in the entry 'model.data' of type EngineData.
56  #This is a wrapper around a pandas.DataFrame data-structure, which is
57  #the entry EngineModel.data. Hence we use the method DataFrame.plot, which
58  #is a convenient interface for plotting of the data inside the DataFrame instance
59
60  #Pressure
61  model.data.data.plot(\
62      x="CA", y="pBar",                          #x and y variables
63      c="k", ylabel="p [bar]", xlabel="[CAD]",   #Formatting
64      ax=axP,                                    #Axes
65      legend=False)                              #No legend
66
67  #Rate of heat release (ROHR)
68  model.data.data.plot(\
69      x="CA", y="ROHR",                          #x and y variables
70      c="k", ls="--", ylabel="ROHR [J/CA]",      #Formatting
71      ax=axRohr,                                 #Axes
72      legend=False)                              #No legend
73
74  #Adjust axes and limits
75  plt.tight_layout()
76  axP.set_xlim((-30,30))  #x axis
77  axP.set_ylim((-10,40))  #pressure
78  axRohr.set_ylim((0,100)) #ROHR
79
80  #Show the figure
81  plt.show()
```

Plotting results

sparkIgnitionExample/main.py

```
47      'figure.figsize':(6,12),
48      # 'figure.dpi':10
49  })
50
51  #Create figure and combined axes (pressure lefr, ROHR right)
52  fig, axP = plt.subplots(1,1, figsize=(6,8))
53  axRohr = axP.twinx()
54
55  #Processed data are stored in the entry 'model.data' of type EngineData.
56  #This is a wrapper around a pandas.DataFrame data-structure, which is
57  #the entry EngineModel.data. Hence we use the method DataFrame.plot, which
58  #is a convenient interface for plotting of the data inside the DataFrame instance
59
60  #Pressure
61  model.data.data.plot(\
62      x="CA", y="pBar",                          #x and y variables
63      c="k", ylabel="p [bar]", xlabel="[CAD]",   #Formatting
64      ax=axP,                                    #Axes
65      legend=False)                              #No legend
66
67  #Rate of heat release (ROHR)
68  model.data.data.plot(\
69      x="CA", y="ROHR",                          #x and y variables
70      c="k", ls="--", ylabel="ROHR [J/CA]",      #Formatting
71      ax=axRohr,                                 #Axes
72      legend=False)                              #No legend
73
74  #Adjust axes and limits
75  plt.tight_layout()
76  axP.set_xlim((-30,30))  #x axis
77  axP.set_ylim((-10,40))  #pressure
78  axRohr.set_ylim((0,100)) #ROHR
79
80  #Show the figure
81  plt.show()
```

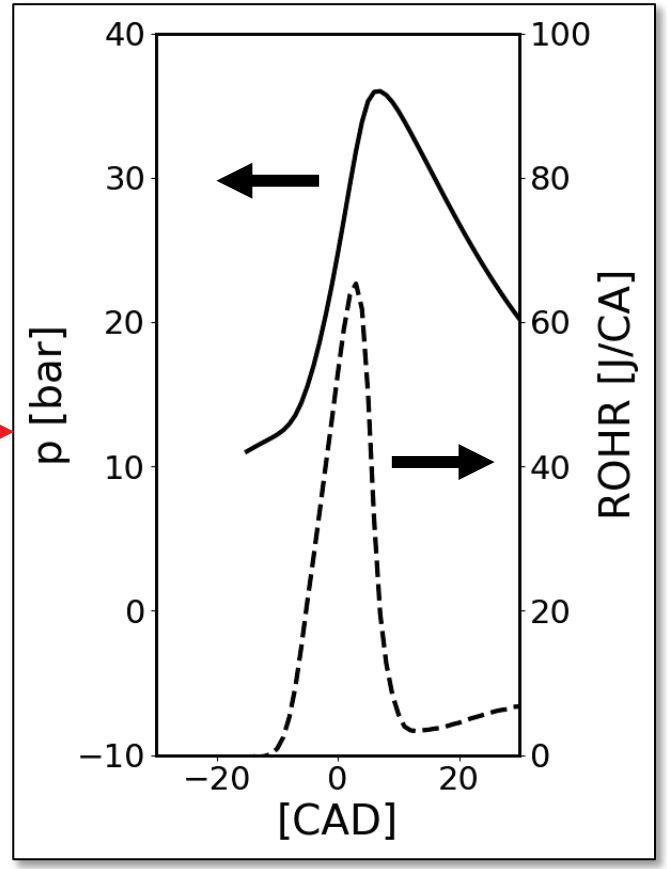
Adjusting the axes and limits

Plotting results

sparkIgnitionExample/main.py

```
47      'figure.figsize':(6,12),
48      # 'figure.dpi':10
49  })
50
51  #Create figure and combined axes (pressure lefr, ROHR right)
52  fig, axP = plt.subplots(1,1, figsize=(6,8))
53  axRohr = axP.twinx()
54
55  #Processed data are stored in the entry 'model.data' of type EngineData.
56  #This is a wrapper around a pandas.DataFrame data-structure, which is
57  #the entry EngineModel.data. Hence we use the method DataFrame.plot, which
58  #is a convenient interface for plotting of the data inside the DataFrame instance
59
60  #Pressure
61  model.data.data.plot(\
62      x="CA", y="pBar",                          #x and y variables
63      c="k", ylabel="p [bar]", xlabel="[CAD]",   #Formatting
64      ax=axP,                                    #Axes
65      legend=False)                              #No legend
66
67  #Rate of heat release (ROHR)
68  model.data.data.plot(\
69      x="CA", y="ROHR",                          #x and y variables
70      c="k", ls="--", ylabel="ROHR [J/CA]",      #Formatting
71      ax=axRohr,                                 #Axes
72      legend=False)                              #No legend
73
74  #Adjust axes and limits
75  plt.tight_layout()
76  axP.set_xlim((-30,30))  #x axis
77  axP.set_ylim((-10,40))  #pressure
78  axRohr.set_ylim((0,100)) #ROHR
79
80  #Show the figure
81  plt.show()
```

Showing the plot



Final remarks

- **Next steps:**
  - **Extension** of the classes to handle different engine configurations (Diesel engines, Wankel, etc…)
  - Implementation of existing workflows into **executable scripts**
  - Development of a **GUI** to simplify user experience

Contact information

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