# **RayPyNG**

Simone Vadilonga, Ruslan Ovsyannikov

## **CONTENTS:**

1	Simulate	1
2	SimulationParams	5
3	RayUIRunner	7
4	PostProcessing	9
Index		13

#### **CHAPTER**

## ONE

## **SIMULATE**

class raypyng.simulate.Simulate(rml=None, hide=False, \*\*kwargs)

A class that takes care of performing the simulations with RAY-UI

```
__init__(rml=None, hide=False, **kwargs) \rightarrow None
```

Initialize the class with a rml file :param rml: string pointing to an rml file with the beamline template, or an RMLFile class object. Defaults to None. :type rml: RMLFile/string, optional :param hide: force hiding of GUI leftovers, xvfb needs to be installed. Defaults to False. :type hide: bool, optional

#### Raises

**Exception** – If the rml file is not defined an exception is raised

#### \_\_weakref\_\_

list of weak references to the object (if defined)

#### property analyze

Turn on or off the RAY-UI analysis of the results. The analysis of the results takes time, so turn it on only if needed

#### Returns

True: analysis on, False: analysis off

## Return type

bool

### property exports

The files to export once the simulation is complete. for a list of possible files check self.possible\_exports and self.possible\_exports\_without\_analysis.

It is expected a list of dictionaries, and for each dictionary the key is the element to be exported and the valuee are the files to be exported

#### property params

The parameters to scan, as a list of dictionaries. For each dictionary the keys are the parameters elements of the beamline, and the values are the values to be assigned.

#### property path

The path where to execute the simlations

#### Returns

by default the path is the current path from which the program is executed

## Return type

string

#### property possible\_exports

A list of the files that can be exported by RAY-UI

#### Returns

list of the names of the possible exports for RAY-UI

#### **Return type**

list

#### property possible\_exports\_without\_analysis

A list of the files that can be exported by RAY-UI when the analysis option is turned off

#### **Returns**

list of the names of the possible exports for RAY-UI when analysis is off

#### Return type

list

#### property raypyng\_analysis

Turn on or off the RAYPyNG analysis of the results.

#### Returns

True: analysis on, False: analysis off

#### Return type

bool

#### property repeat

The simulations can be repeated an arbitrary number of times If the statitcs are not good enough using 2 millions of rays is suggested to repeat them instead of increasing the number of rays

#### Returns

the number of repetition of the simulations, by default is 1

#### Return type

int

## property rml

RMLFile object instantiated in init

## rml\_list()

This function creates the folder structure and the rml files to simulate. It requires the param to be set. Useful if one wants to create the simulation files for a manual check before starting the simulations.

```
run(recipe=None, /, multiprocessing=True, force=False)
```

This method starts the simulations, params and exports need to be defined.

#### **Parameters**

- recipe (SimulationRecipe, optional) If using a recipee pass it as a parameter. Defaults to None.
- multiprocessing (boolint, optional) If True all the cpus are used. If an integer n is provided, n cpus are used. Defaults to True.
- **force** (*bool*, *optional*) If True all the similations are performed, even if the export files already exist. If False only the similations for which are missing some exports are performed. Defaults to False.

## ${\tt save\_parameters\_to\_file}(\mathit{dir})$

save all the user input parameters to file. It takes the values from the SimulationParams class

#### **Parameters**

**dir** (*str*) – the folder where to save the parameters

## property simulation\_name

A string to append to the folder where the simulations will be executed.

## **SIMULATION PARAMS**

class raypyng.simulate.SimulationParams(rml=None, param\_list=None, \*\*kwargs)

A class that takes care of the simulations parameters, makes sure that they are written correctly, and returns the the list of simulations that is requested by the user.

```
\begin{tabular}{ll} $\_\_init\_\_(rml=None, param\_list=None, **kwargs) \to None \\ $\_\_summary\_$ \end{tabular}
```

#### **Parameters**

- **rml** (*RMLFile/string*, *optional*) string pointing to an rml file with the beamline template, or an RMLFile class object. Defaults to None.
- param\_list (list, optional) list of dictionaries containing the parameters and values to simulate. Defaults to None.

### \_\_weakref\_\_

list of weak references to the object (if defined)

```
_calc_loop(verbose: bool = True)
```

Calculate the simulations loop

#### Returns

idependent and dependent parameters self.simulations\_param\_list (list): parameters values for each simulation loop

#### Return type

self.param\_to\_simulate (list)

#### \_check\_if\_enabled(param)

Check if a parameter is enabled

#### **Parameters**

param (RML object) - an parameter to simulate

#### **Returns**

True if the parameter is enabled, False otherwise

#### Return type

(bool)

## \_check\_param()

Check that self.param is a list of dictionaries, and convert the items of the dictionaries to lists, otherwise raise an exception.

#### \_enable\_param(param)

Set enabled to True in a beamline object, and auto to False

#### **Parameters**

param (RML object) - beamline object

```
_extract_param(verbose: bool = False)
```

Parse self.param and extract dependent and independent parameters

#### **Parameters**

**verbose** (bool, optional) – If True print the returned objects. Defaults to False.

#### **Returns**

indieendent parameter values self.ind\_par (list): independent parameters self.dep\_param\_dependency (dict): dictionary of dependencies self.dep\_value\_dependency (list): dictionaries of dependent values self.dep\_par (list): dependent parameters

#### Return type

self.ind\_param\_values (list)

#### \_write\_value\_to\_param(param, value)

Write a value to a parameter, making sure enable is T and auto is F

#### **Parameters**

- param (RML object) beamline object
- value (str, int, float) the value to set the beamline object to

#### property params

The parameters to scan, as a list of dictionaries. For each dictionary the keys are the parameters elements of the beamline, and the values are the values to be assigned.

#### property rml

RMLFile object instantiated in init

## THREE

## **RAYUIRUNNER**

```
class raypyng.runner.RayUIRunner(ray_path=None, ray_binary='rayui.sh', background=True, hide=False)
      RayUIRunner class implements all logic to start a RayUI process
      \_detect_ray_path() \rightarrow str
           Internal function to autodetect installation path of RayUI
                Raises
                    RayPyRunnerError – is case no ray installations can be detected
                Returns
                    string with the detected ray installation path
                Return type
                    str
      \__init\_(ray_path=None, ray_binary='rayui.sh', background=True, hide=False) \rightarrow None
      __weakref__
           list of weak references to the object (if defined)
      _{\mathbf{readline}}() \rightarrow \operatorname{str}
           read a line from the stdout of the process and convert to a string
                    line read from the input
                Return type
      _write(instr: str, endline=\n')
           Write command to RayUI interface
                Parameters
                    • instr (str) – _description_
                    • endline (str, optional) – _description_. Defaults to endline character.
                Raises
                    RayPyRunnerError – _description_
      property isrunning
           Check weather a process is running and rerutn a boolean
```

returns True if the process is running, otherwise False

```
Return type
```

bool

kill()

kill a RAY-UI process

property pid

Get process id of the RayUI process

Returns

PID of the process if it running, None otherwise

Return type

\_type\_

run()

Open one instance of RAY-UI using subprocess

Raises

RayPyRunnerError – if the RAY-UI executable is not found raise an error

## **POSTPROCESSING**

```
class raypyng.postprocessing.PostProcess
     class to post-process the data. At the moment works only if the exported data are RawRaysOutgoing
     __init__() \rightarrow None
     __weakref__
          list of weak references to the object (if defined)
     _extract_bandwidth_fwhm(rays_bw: array)
           calculate the fwhm of the rays_bw.
               Parameters
                   (np (rays_bw) – array): the energy of the x-rays
               Returns
                   fwhm
               Return type
                   float
     _extract_focus_fwhm(rays_pos: array)
          calculate the fwhm of rays_pos
               Parameters
                   rays_pos (np.array) – contains positions of the x-rays
               Returns
                   fwhm
               Return type
                   float
     _extract_intensity(rays: array)
           calculate how many rays there are
               Parameters
                   rays (np. array) - contains rays information
     _list_files(dir_path: str, end_filename: str)
          List all the files in dir_path ending with end_filename
               Parameters
                   • dir_path (str) - path to a folder
```

• **end\_filename** (*str*) – the listed files end with end\_filename

#### Returns

list of files in dir\_path ending eith end\_filename

#### Return type

res (list)

#### \_load\_file(filepath)

Load a .npy file and returns the array

#### **Parameters**

**filepath** (*str*) – the path to the file to load

#### Returns

The loaded numpy array

#### Return type

arr (np.array)

 $_{ extbf{save_file}}(filename: str, array: array, header: Optional[str] = None)$ 

This function is used to save files,

#### **Parameters**

- **filename** (str) file name(path)
- array (np. array) array to save
- **header** (*str*) header for the file

 $cleanup(dir\_path: Optional[str] = None, repeat: int = 1, exp\_elements: Optional[list] = None)$ 

This functions reads all the temporary files created by self.postptocess\_RawRays() saves one file for each exported element in dir\_path, and deletes the temporary files. If more than one round of simulations was done, the values are averaged.

#### **Parameters**

- **dir\_path** (*str*, *optional*) The path to the folder to cleanup. Defaults to None.
- **repeat** (*int*, *optional*) number of rounds of simulations. Defaults to 1.
- **exp\_elements** (*list*, *optional*) the exported elements names as str. Defaults to None.

#### extract\_nrays\_from\_source(rml\_filename)

Extract photon flux from rml file, find source automatically

#### **Parameters**

**rml\_filename** (str) – the rml file to use to extract the photon flux

#### Returns

the photon flux

#### Return type

stı

The method looks in the folder dir\_path for a file with the filename: filename = os.path.join(dir\_path,sim\_number+exported\_element + '-' + exported\_object+'.csv') for each file it calculates the number of rays, the bandwidth, and the horizontal and vertical focus size, it saves it in an array that is composed by [n\_rays,bandwidth,hor\_focus,vert\_focus], that is then saved to os.path.join(dir\_path, sim\_number+exported\_element+'\_analyzed\_rays.npy') :param exported\_element:

a list of containing the exported elements name as str. Defaults to None. :type exported\_element: list, optional :param exported\_object: the exported opbject, tested only with RawRaysOutgoing. Defaults to None. :type exported\_object: str, optional :param dir\_path: the folder where the file to process is located. Defaults to None. :type dir\_path: str, optional :param sim\_number: the prefix of the file, that is the simulation number with a \_prepended, ie "0\_". Defaults to None. :type sim\_number: str, optional

## **INDEX**

Symbols	method), 10
detect_ray_path() (raypyng.runner.RayUIRunner	_write() (raypyng.runner.RayUIRunner method), 7
method), 7	_write_value_to_param()
init() (raypyng.postprocessing.PostProcess method), 9	(raypyng.simulate.SimulationParams method),
init() (raypyng.runner.RayUIRunner method), 7	Α
init() (raypyng.simulate.Simulate method), 1	
init() (raypyng.simulate.SimulationParams	analyze (raypyng.simulate.Simulate property), 1
method), 5	C
weakref (raypyng.postprocessing.PostProcess at-	
tribute), 9	cleanup() (raypyng.postprocessing.PostProcess
weakref (raypyng.runner.RayUIRunner attribute),	method), 10
7	E
weakref (raypyng.simulate.Simulate attribute), 1	exports (raypyng.simulate.Simulate property), 1
weakref (raypyng.simulate.SimulationParams at-	extract_nrays_from_source()
tribute), 5	(raypyng.postprocessing.PostProcess method),
_calc_loop() (raypyng.simulate.SimulationParams	10
method), 5	
_check_if_enabled()	I
(raypyng.simulate.SimulationParams method), 5	${\tt isrunning}\ (\textit{raypyng.runner.RayUIRunner property}), 7$
_check_param() (raypyng.simulate.SimulationParams	K
method), 5	kill() (raypyng.runner.RayUIRunner method), 8
_enable_param() (raypyng.simulate.SimulationParams	
method), 5	P
_extract_bandwidth_fwhm()	params (raypyng.simulate.Simulate property), 1
(raypyng.postprocessing.PostProcess method),	params (raypyng.simulate.SimulationParams property),
9	6
_extract_focus_fwhm()	path (raypyng.simulate.Simulate property), 1
(raypyng.postprocessing.PostProcess method),	pid (raypyng.runner.RayUIRunner property), 8
_extract_intensity()	possible_exports (raypyng.simulate.Simulate prop-
(raypyng.postprocessing.PostProcess method),	erty), 1
9	possible_exports_without_analysis
_extract_param() (raypyng.simulate.SimulationParams	(raypyng.simulate.Simulate property), 2
method), 6	PostProcess (class in raypyng.postprocessing), 9
_list_files() (raypyng.postprocessing.PostProcess	<pre>postprocess_RawRays()</pre>
method), 9	(raypyng.postprocessing.PostProcess method),
_load_file() (raypyng.postprocessing.PostProcess	10
method), 10	R
_readline() (raypyng.runner.RayUIRunner method), 7	raypyng_analysis (raypyng.simulate.Simulate prop-
_save_file() (raypyng.postprocessing.PostProcess	erty), 2

```
RayUIRunner (class in raypyng.runner), 7
repeat (raypyng.simulate.Simulate property), 2
rml (raypyng.simulate.Simulate property), 2
rml (raypyng.simulate.SimulationParams property), 6
rml_list() (raypyng.simulate.Simulate method), 2
run() (raypyng.runner.RayUIRunner method), 8
run() (raypyng.simulate.Simulate method), 2
S
save_parameters_to_file()
```

```
(raypyng.simulate.Simulate method), 2
Simulate (class in raypyng.simulate), 1
{\tt simulation\_name} \quad (\textit{raypyng.simulate.Simulate} \quad \textit{prop-}
           erty), 3
SimulationParams (class in raypyng.simulate), 5
```

14 Index