
Cortix Documentation

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1.1 cortix_main

class cortix_main.**Cortix** (*use_mpi=False, splash=False*)

Bases: `object`

Cortix main class definition

The typical Cortix workflow:

1. Create the object
2. Add and connect modules
3. Run the simulation

use_mpi

bool – True for MPI, False for multiprocessing

splash

bool – Show the Cortix splash image

comm

mpi4py.MPI.Intracomm – MPI.COMM_WORLD (if using MPI else None)

rank

int – The current MPI rank (if using MPI else None)

size

int – size of the group associated with MPI.COMM_WORLD

__del__ ()

Destructs a Cortix simulation object

Warning: By the time the body of this function is executed, the machinery of variables may have been deleted already. For example, *logging* is no longer there; do the least amount of work here.

__init__ (*use_mpi=False, splash=False*)

Construct a Cortix simulation object

Parameters

- **use_mpi** (*bool*) – True for MPI, False for multiprocessing
- **splash** (*bool*) – Show the Cortix splash image

add_module (*m*)

Add a Module object to the Cortex Simulation

Parameters *m* (`Module`) – The Module object to be added

draw_network (*file_name='network.png', dpi=220*)

Draws the networkx Module network graph to an image

Parameters

- **file_name** (*str, optional*) – The resulting network diagram output file name
- **dpi** (*int, optional*) – dpi used for generating the network image

get_modules ()

Return a list of all the Cortex modules from the master process

If the *run()* method has completed, the list is updated with data from the other processes.

Returns *modules* – The list of modules in the Cortex simulation

Return type `list(Module)`

get_network ()

Constructs and returns a the module network

Returns a networkx MultiGraph representation of the module network.

Returns *g*

Return type `networkx.classes.multigraph.MultiGraph`

run ()

Run the Cortex simulation

This function concurrently executes the `cortex.src.module.run` function for each module in the simulation. Modules are run using either MPI or Multiprocessing, depending on the user configuration.

1.2 module module

class `module.Module`

Bases: `object`

Cortex module super class

This class provides facilities for creating modules within the Cortex network. Cortex will map one object of this class to either a Multiprocessing or MPI process depending on the user's configuration.

Note: This class is to be inherited by every Cortex module. In order to execute, modules *must* override the *run* method, which will be executed during the simulation

name

str – A name given to the instance. Default is *None*.

port_names_expected

list(str), None – A list of names of ports expected in the module. This will be compared to port names during runtime to check against the intended use of the module.

state

any – Any *pickle-able* data structure to be passed in a *multiprocessing.Queue* to the parent process or to be gathered in the root MPI process. Default is *None*.

use_mpi

bool – True for MPI, false for Multiprocessing

ports

list(Port) – A list of ports contained by the module

__init__()

Module super class constructor

This must be called in the constructor of every Cortix module like so:

```
>> super().__init__()
```

connect (*port_name_or_module*, *to_other_port=None*)

Connect two modules using ports corresponding to their name

Parameters

- **port_name_or_module** (*str*, *Module*) – Either a *port* name or a *Module* can be given. In the latter case the *name* attribute of the module will be used to get the *port* of the module passed. This port will be connected to the port of the calling object.
- **to_other_port** (*Port*) – A *port* object to connect to. This must be *None* or absent if the first argument is a *Module*.

get_port (*name*)

Get port by name; if it does not exist, create one.

Parameters **name** (*str*) – The name of the port to get

Returns **port** – The port object with the corresponding name

Return type *Port*

recv (*port*)

Receive data from a given port

Warning: This function will block until data is available

Parameters **port** (*Port*, *str*) – A *Port* object to send the data through, or its string name

Returns **data** – The data received through the port

Return type any

run (**args*)

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with *run(self)* or *run(self, *args)* as long as *self.state = None*. If *self.state* points to anything but *None*, the user must use **run(self, *args)*.

Notes

When in multiprocessing, **args* has two elements: *comm_idx* and *comm_state*. To pass back the state of the module, the user should insert the provided index *comm_idx* and the *state* into the queue as follows:

if not self.use_mpi:

try: pickle.dumps(self.state)

```
except pickle.PicklingError: args[1].put((arg[0],None))
```

```
else: args[1].put((arg[0],self.state))
```

at the bottom of the user defined run() function.

Warning: This function must be overridden by all Cortex modules

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library *state_comm* must have the module's *self.state* in it. That is, *state_comm.put((idx_comm,self.state))* must be the last command in the method before *return*. In addition, *self.state* must be *pickle-able*.

send (*data, port*)

Send data through a given port.

Parameters

- **data** (*any*) – The data being sent out - must be pickleable
- **port** (*Port, str*) – A Port object to send the data through, or its string name

1.3 port module

class port.Port (*name=None, use_mpi=False*)

Bases: *object*

Provides a method of communication between modules

The Port class provides an interface for creating ports and connecting them to other ports for the purpose of data transfer. Data exchange takes place by send and/or receive calls on a given port. The concept of a port is that of a data transfer “interaction.” This can be one- or two-way with sends and receives. A port is connected to only one other port; as two ends of a pipe are connected.

id

int

name

string

use_mpi

bool

__eq__ (*other*)

Check for port equality

__init__ (*name=None, use_mpi=False*)

Constructs a Port object

Parameters

- **name** (*str*) – The name of the Port object
- **use_mpi** (*bool*) – True for MPI, False for Multiprocessing

`__repr__()`

Port name representation

connect (*port*)

Connect this port to another port

Ports must be connected for data to flow between them.

Parameters **port** (`Port`) – A Port object to connect to

recv ()

Receive data from the connected port.

Warning: This function will block if no data has been sent yet.
--

Returns **data**

Return type `any`

send (*data*, *tag=None*)

Send data to the connected port.

If the sending port is not connected do nothing.

Parameters

- **data** (*any*) – This data must be pickleable
- **tag** (*int*, *optional*) – MPI tag used in sending data

EXAMPLES

2.1 adjudication module

class adjudication.**Adjudication** (*n_groups=1, pool_size=0.0*)

Bases: cortix.src.module.Module

Adjudication Cortix module used to model criminal group population in an adjudication system.

Notes

These are the *port* names available in this module to connect to respective modules: *probation*, *jail*, *arrested*, *prison*, and *community*. See instance attribute *port_names_expected*.

__init__ (*n_groups=1, pool_size=0.0*)

Parameters

- **n_groups** (*int*) – Number of groups in the population.
- **pool_size** (*float*) – Upperbound on the range of the existing population groups. A random value from 0 to the upperbound value will be assigned to each group.

run (**args*)

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with *run(self)* or *run(self, *args)* as long as *self.state = None*. If *self.state* points to anything but *None*, the user must use *run(self, *args)*.

Notes

When in multiprocessing, **args* has two elements: *comm_idx* and *comm_state*. To pass back the state of the module, the user should insert the provided index *comm_idx* and the *state* into the queue as follows:

if not self.use_mpi:

try: pickle.dumps(self.state)

except pickle.PicklingError: args[1].put((arg[0],None))

else: args[1].put((arg[0],self.state))

at the bottom of the user defined run() function.

Warning: This function must be overridden by all Cortix modules

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library *state_comm* must have the module's *self.state* in it. That is, *state_comm.put((idx_comm,self.state))* must be the last command in the method before *return*. In addition, *self.state* must be *pickle-able*.

2.2 arrested module

class arrested.**Arrested** (*n_groups=1, pool_size=0.0*)

Bases: *cortix.src.module.Module*

Arrested Cortix module used to model criminal group population in an arrested system.

Notes

These are the *port* names available in this module to connect to respective modules: *probation*, *adjudication*, *jail*, and *community*. See instance attribute *port_names_expected*.

__init__ (*n_groups=1, pool_size=0.0*)

Parameters

- **n_groups** (*int*) – Number of groups in the population.
- **pool_size** (*float*) – Upperbound on the range of the existing population groups. A random value from 0 to the upperbound value will be assigned to each group.

run (**args*)

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with *run(self)* or *run(self, *args)* as long as *self.state = None*. If *self.state* points to anything but *None*, the user must use *run(self, *args)*.

Notes

When in multiprocessing, **args* has two elements: *comm_idx* and *comm_state*. To pass back the state of the module, the user should insert the provided index *comm_idx* and the *state* into the queue as follows:

if not self.use_mpi:

try: *pickle.dumps(self.state)*

except pickle.PicklingError: *args[1].put((arg[0],None))*

else: *args[1].put((arg[0],self.state))*

at the bottom of the user defined *run()* function.

Warning: This function must be overridden by all Cortex modules

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library *state_comm* must have the module's *self.state* in it. That is, *state_comm.put((idx_comm,self.state))* must be the last command in the method before *return*. In addition, *self.state* must be *pickle-able*.

2.3 community module

```
class community.Community(n_groups=1, maturity_rate=0.00011574074074074075, of-
                           fender_pool_size=0.0)
Bases: cortix.src.module.Module
```

Community Cortex module used to model criminal group population in a community system. Community here is the system at large with all possible adult individuals included in a society.

Notes

These are the *port* names available in this module to connect to respective modules: *probation*, *adjudication*, *jail*, *prison*, *arrested*, and *parole*. See instance attribute *port_names_expected*.

```
__init__(n_groups=1, maturity_rate=0.00011574074074074075, offender_pool_size=0.0)
```

Parameters

- **n_groups** (*int*) – Number of groups in the population.
- **maturity_rate** (*float*) – Rate of individuals reaching the adult age (SI) unit. Default: 10 per day.
- **offender_pool_size** (*float*) – Upperbound on the range of the existing population groups. A random value from 0 to the upperbound value will be assigned to each group.

```
run(*args)
```

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with *run(self)* or *run(self, *args)* as long as *self.state = None*. If *self.state* points to anything but *None*, the user must use **run(self, *args)*.

Notes

When in multiprocessing, **args* has two elements: *comm_idx* and *comm_state*. To pass back the state of the module, the user should insert the provided index *comm_idx* and the *state* into the queue as follows:

if not self.use_mpi:

try: pickle.dumps(self.state)

except pickle.PicklingError: args[1].put((arg[0],None))

else: args[1].put((arg[0],self.state))

at the bottom of the user defined `run()` function.

Warning: This function must be overridden by all Cortix modules

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library *state_comm* must have the module's *self.state* in it. That is, *state_comm.put((idx_comm,self.state))* must be the last command in the method before *return*. In addition, *self.state* must be *pickle-able*.

2.4 dataplot module

```
class dataplot.DataPlot
    Bases: cortix.src.module.Module

    plot_data()

    recv_data(port)
        Keep listening on the port and receiving data.

    run(*args)
        Spawn a thread to handle each port connection.
```

2.5 droplet module

```
class droplet.Droplet
    Bases: cortix.src.module.Module

    Droplet Cortix module used to model very simple fluid-particle interactions.
```

Notes

Port names used in this module: *external-flow* exchanges data with any other module that provides information about the flow outside the droplet, *visualization* sends data to a visualization module.

```
__init__()

initial_time
    float

end_time
    float

time_step
    float

show_time
    tuple – Two-element tuple, (bool,float), True will print to standard output.
```

run (*args)

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with *run(self)* or *run(self, *args)* as long as *self.state = None*. If *self.state* points to anything but *None*, the user must use *run(self, *args)*.

Notes

When in multiprocessing, **args* has two elements: *comm_idx* and *comm_state*. To pass back the state of the module, the user should insert the provided index *comm_idx* and the *state* into the queue as follows:

if not self.use_mpi:

try: pickle.dumps(self.state)

except pickle.PicklingError: args[1].put((arg[0],None))

else: args[1].put((arg[0],self.state))

at the bottom of the user defined run() function.

Warning: This function must be overridden by all Cortix modules

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library *state_comm* must have the module's *self.state* in it. That is, *state_comm.put((idx_comm,self.state))* must be the last command in the method before *return*. In addition, *self.state* must be *pickle-able*.

2.6 dummy_module module

class dummy_module.DummyModule

Bases: cortix.src.module.Module

run ()

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with *run(self)* or *run(self, *args)* as long as *self.state = None*. If *self.state* points to anything but *None*, the user must use *run(self, *args)*.

Notes

When in multiprocessing, **args* has two elements: *comm_idx* and *comm_state*. To pass back the state of the module, the user should insert the provided index *comm_idx* and the *state* into the queue as follows:

if not self.use_mpi:

try: pickle.dumps(self.state)

```

    except pickle.PicklingError: args[1].put((arg[0],None))
    else: args[1].put((arg[0],self.state))

```

at the bottom of the user defined run() function.

Warning: This function must be overridden by all Cortex modules

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library *state_comm* must have the module's *self.state* in it. That is, *state_comm.put((idx_comm,self.state))* must be the last command in the method before *return*. In addition, *self.state* must be *pickle-able*.

```

class dummy_module.DummyModule2
    Bases: cortex.src.module.Module

```

```

run()

```

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with *run(self)* or *run(self, *args)* as long as *self.state = None*. If *self.state* points to anything but *None*, the user must use *run(self, *args)*.

Notes

When in multiprocessing, **args* has two elements: *comm_idx* and *comm_state*. To pass back the state of the module, the user should insert the provided index *comm_idx* and the *state* into the queue as follows:

```

if not self.use_mpi:
    try: pickle.dumps(self.state)
    except pickle.PicklingError: args[1].put((arg[0],None))
    else: args[1].put((arg[0],self.state))

```

at the bottom of the user defined run() function.

Warning: This function must be overridden by all Cortex modules

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library *state_comm* must have the module's *self.state* in it. That is, *state_comm.put((idx_comm,self.state))* must be the last command in the method before *return*. In addition, *self.state* must be *pickle-able*.

2.7 jail module

class jail.Jail(*n_groups=1, pool_size=0.0*)

Bases: cortix.src.module.Module

Jail Cortix module used to model criminal group population in a jail.

Notes

These are the *port* names available in this module to connect to respective modules: *probation*, *adjudication*, *arrested*, *prison*, and *community*. See instance attribute *port_names_expected*.

__init__(*n_groups=1, pool_size=0.0*)

Parameters

- **n_groups** (*int*) – Number of groups in the population.
- **pool_size** (*float*) – Upperbound on the range of the existing population groups. A random value from 0 to the upperbound value will be assigned to each group.

run(**args*)

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with *run(self)* or *run(self, *args)* as long as *self.state = None*. If *self.state* points to anything but *None*, the user must use *run(self, *args)*.

Notes

When in multiprocessing, **args* has two elements: *comm_idx* and *comm_state*. To pass back the state of the module, the user should insert the provided index *comm_idx* and the *state* into the queue as follows:

```
if not self.use_mpi:
    try: pickle.dumps(self.state)
    except pickle.PicklingError: args[1].put((arg[0],None))
    else: args[1].put((arg[0],self.state))
```

at the bottom of the user defined *run()* function.

Warning: This function must be overridden by all Cortix modules

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library *state_comm* must have the module's *self.state* in it. That is, *state_comm.put((idx_comm,self.state))* must be the last command in the method before *return*. In addition, *self.state* must be *pickle-able*.

2.8 parole module

class parole.**Parole** (*n_groups=1, pool_size=0.0*)

Bases: cortix.src.module.Module

Parole Cortix module used to model criminal group population in a parole system.

Notes

These are the *port* names available in this module to connect to respective modules: *prison* and *community*. See instance attribute *port_names_expected*.

run (**args*)

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with *run(self)* or *run(self, *args)* as long as *self.state = None*. If *self.state* points to anything but *None*, the user must use *run(self, *args)*.

Notes

When in multiprocessing, **args* has two elements: *comm_idx* and *comm_state*. To pass back the state of the module, the user should insert the provided index *comm_idx* and the *state* into the queue as follows:

if not self.use_mpi:

try: pickle.dumps(self.state)

except pickle.PicklingError: args[1].put((arg[0],None))

else: args[1].put((arg[0],self.state))

at the bottom of the user defined run() function.

<p>Warning: This function must be overridden by all Cortix modules</p>

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library *state_comm* must have the module's *self.state* in it. That is, *state_comm.put((idx_comm,self.state))* must be the last command in the method before *return*. In addition, *self.state* must be *pickle-able*.

2.9 plot_data module

class plot_data.**PlotData**

Bases: cortix.src.module.Module

run ()

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with `run(self)` or `run(self, *args)` as long as `self.state = None`. If `self.state` points to anything but `None`, the user must use `run(self, *args)`.

Notes

When in multiprocessing, `*args` has two elements: `comm_idx` and `comm_state`. To pass back the state of the module, the user should insert the provided index `comm_idx` and the `state` into the queue as follows:

```
if not self.use_mpi:
    try: pickle.dumps(self.state)
    except pickle.PicklingError: args[1].put((arg[0],None))
    else: args[1].put((arg[0],self.state))
```

at the bottom of the user defined `run()` function.

Warning: This function must be overridden by all Cortix modules
--

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library `state_comm` must have the module's `self.state` in it. That is, `state_comm.put((idx_comm,self.state))` must be the last command in the method before `return`. In addition, `self.state` must be *pickle-able*.

2.10 prison module

```
class prison.Prison(n_groups=1, pool_size=0.0)
```

Bases: `cortix.src.module.Module`

Prison Cortix module used to model criminal group population in a prison.

Notes

These are the *port* names available in this module to connect to respective modules: *parole*, *adjudication*, *jail*, and *community*. See instance attribute `port_names_expected`.

```
__init__(n_groups=1, pool_size=0.0)
```

Parameters

- **n_groups** (*int*) – Number of groups in the population.
- **pool_size** (*float*) – Upperbound on the range of the existing population groups. A random value from 0 to the upperbound value will be assigned to each group.

```
run(*args)
```

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with `run(self)` or `run(self, *args)` as long as `self.state = None`. If `self.state` points to anything but `None`, the user must use `run(self, *args)`.

Notes

When in multiprocessing, `*args` has two elements: `comm_idx` and `comm_state`. To pass back the state of the module, the user should insert the provided index `comm_idx` and the `state` into the queue as follows:

```
if not self.use_mpi:
    try: pickle.dumps(self.state)
    except pickle.PicklingError: args[1].put((arg[0],None))
    else: args[1].put((arg[0],self.state))
```

at the bottom of the user defined `run()` function.

Warning: This function must be overridden by all Cortex modules
--

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library `state_comm` must have the module's `self.state` in it. That is, `state_comm.put((idx_comm,self.state))` must be the last command in the method before `return`. In addition, `self.state` must be *pickle-able*.

2.11 probation module

```
class probation.Probation (n_groups=1, pool_size=0.0)
```

Bases: `cortex.src.module.Module`

Probation Cortex module used to model criminal group population in a probation.

Notes

These are the *port* names available in this module to connect to respective modules: *adjudication*, *jail*, *arrested*, and *community*. See instance attribute `port_names_expected`.

```
__init__ (n_groups=1, pool_size=0.0)
```

Parameters

- **n_groups** (*int*) – Number of groups in the population.
- **pool_size** (*float*) – Upperbound on the range of the existing population groups. A random value from 0 to the upperbound value will be assigned to each group.

```
run (*args)
```

Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with `run(self)` or `run(self, *args)` as long as `self.state = None`. If `self.state` points to anything but `None`, the user must use `run(self, *args)`.

Notes

When in multiprocessing, `*args` has two elements: `comm_idx` and `comm_state`. To pass back the state of the module, the user should insert the provided index `comm_idx` and the `state` into the queue as follows:

```
if not self.use_mpi:
    try: pickle.dumps(self.state)
    except pickle.PicklingError: args[1].put((arg[0],None))
    else: args[1].put((arg[0],self.state))
```

at the bottom of the user defined `run()` function.

Warning: This function must be overridden by all Cortex modules
--

Parameters

- **comm_idx** (*int*) – Index of the state in the communication queue.
- **comm_state** (*multiprocessing.Queue*) – When using the Python *multiprocessing* library `state_comm` must have the module's `self.state` in it. That is, `state_comm.put((idx_comm,self.state))` must be the last command in the method before `return`. In addition, `self.state` must be *pickle-able*.

2.12 run_droplet_a module

This example uses two modules instantiated many times. This example can be executed with MPI (if `mpi4py` is available) or with the Python multiprocessing library. These choices are made by variables listed below in the executable portion of this run file.

To run this case using MPI you should compute the number of processes as follows:

$$nprocs = n_droplets + 1 \text{ vortex} + 1 \text{ cortex}$$

then issue the MPI run command as follows (replace `nprocs` with a number):

```
mpiexec -n nprocs run_droplet.py
```

To run this case with the Python multiprocessing library, just run this file at the command line as

```
run_droplet.py
```

2.13 run_droplet_b module

This example uses three modules instantiated many times in two different networks. Each network configuration uses a different amount of module instances and a different network topology. This example can be executed with MPI (if `mpi4py` is available) or with the Python multiprocessing library. These choices are made by variables listed below in the executable portion of this run file.

2.13.1 Single Plot

The first network case is named “single plot”. Here one DataPlot module is connected to all Droplet modules. To run this case using MPI you should compute the number of processes as follows:

$$nprocs = n_droplets + 1 \text{ vortex} + 1 \text{ data_plot} + 1 \text{ cortix}$$

then issue the MPI run command as follows (replace *nprocs* with a number):

```
mpiexec -n nprocs run_droplet.py
```

To run this case with the Python multiprocessing library, just run this file at the command line as

```
run_droplet.py
```

2.13.2 Multiple Plot

The second network case is named “multiple plot”. Here each Droplet is connected to an instance of the DataPlot module, therefore many more nodes are added to the network when compared to the first network case. To run this case using MPI compute

$$nprocs = 2 * n_droplets + 1 \text{ vortex} + 1 \text{ cortix}$$

then issue the MPI run command as follows (replace *nprocs*:

```
mpiexec -n nprocs run_droplet.py
```

To run this case with the Python multiprocessing library, just run this file at the command line as

```
run_droplet.py
```

2.14 run_justice module

Crimninal justice example in progress.

2.15 vortex module

```
class vortex.Vortex
```

```
    Bases: cortix.src.module.Module
```

```
    Vortex module used to model fluid flow using Cortix.
```

Notes

Any *port* name and any number of ports are allowed.

```
__init__()
```

```
    initial_time
```

```
        float
```

```
    end_time
```

```
        float
```

time_step
float

show_time
tuple – Two-element tuple, (bool,float), True will print to standard output.

compute_velocity (time, position)
Compute the vortex velocity at the given external position using a vortex flow model

Parameters

- **time** (float) – Time in SI unit.
- **position** (numpy.ndarray(3)) – Spatial position in SI unit.

Returns vortex_velocity

Return type numpy.ndarray(3)

plot_velocity (time=None)
Plot the vortex velocity as a function of height.

run ()
Module run function

Run method with an option to pass data back to the parent process when running in Python multiprocessing mode. If the user does not want to share data with the parent process, this function can be overridden with *run(self)* or *run(self, *args)* as long as *self.state = None*. If *self.state* points to anything but *None*, the user must use *run(self, *args)*.

Notes

When in multiprocessing, **args* has two elements: *comm_idx* and *comm_state*. To pass back the state of the module, the user should insert the provided index *comm_idx* and the *state* into the queue as follows:

```
if not self.use_mpi:
    try: pickle.dumps(self.state)
    except pickle.PicklingError: args[1].put((arg[0],None))
    else: args[1].put((arg[0],self.state))
```

at the bottom of the user defined run() function.

<p>Warning: This function must be overridden by all Cortix modules</p>

Parameters

- **comm_idx** (int) – Index of the state in the communication queue.
- **comm_state** (multiprocessing.Queue) – When using the Python *multiprocessing* library *state_comm* must have the module's *self.state* in it. That is, *state_comm.put((idx_comm,self.state))* must be the last command in the method before *return*. In addition, *self.state* must be *pickle-able*.

3.1 actor

This is a simple way to hide the name of species of interest in a simulation. The user would modify and copy this class into the Cortex module of interest and keep it private. Author: Valmor de Almeida dealmeidav@ornl.gov; vfda
Sat Aug 15 13:41:12 EDT 2015

class actor.**Actor** (*name*)

Bases: `object`

See atoms list in Specie.

atoms

Returns the specific nuclides found in the specified chemical.

Returns atoms

Return type `list(str)`

formula

Returns the formula of the chemical in question.

Returns formula

Return type `str`

3.2 fuel_bucket

This FuelBucket class is a container for usage with other plant-level process modules. It is meant to represent a fuel bucket of a metal fuel reactor. ——— ATTENTION: ——— This container uses Phase() for phases (cladding and fuel). Therefore user is responsible to make the “history” of the phases consistent. See Phase() info.

Author: Valmor de Almeida dealmeidav@ornl.gov; vfda

class fuel_bucket.**FuelBucket** (*specs=Empty DataFrame Columns: [] Index: []*)

Bases: `object`

__repr__ ()

Converts to string.

__str__ ()

Converts to string.

cladding_end_thickness

Gets the thickness of the hemispherical cladding end caps that are placed on the top and bottom of the fuel slug, in cm.

Returns `cladding_end_thickness`

Return type `float`

cladding_mass

Returns the total mass of cladding material in the bucket, in grams.

Returns `cladding_mass`

Return type `float`

cladding_phase

Returns the phase history of the cladding.

Returns `cladding_phase`

Return type `dataFrame`

cladding_volume

Returns the total volume of cladding in the bucket, in cm^3 .

Returns `cladding_volume`

Return type `float`

cladding_wall_thickness

Returns the thickness of the cladding wall which is on the outside of every fuel slug, and in between both sections of fuel, in cm.

Returns `cladding_wall_thickness`

Return type `float`

fresh_u235_mass

Returns the total amount of uranium-235 in the bucket, in grams.

Returns `fresh_u235_mass`

Return type `float`

fresh_u238_mass

Returns the total amount of uranium-238 in the bucket, in grams.

Returns `fresh_u238_mass`

Return type `float`

fresh_u_mass

Returns the total amount of uranium in the bucket, in grams.

Returns `fresh_u_mass`

Return type `float`

fuel_enrichment

Returns the enrichment of the fuel slugs in the bucket, in %.

Returns `fuel_enrichment`

Return type `float`

fuel_mass

Returns the total mass of fuel in the solid phase in the bucket.

Returns `fuel_mass`

Return type `float`

fuel_mass_unit

Returns the unit that is used to measure the mass of fuel in the bucket.

Returns `fuel_mass_unit`

Return type `str`

fuel_phase

Returns the phase history of the fuel.

Returns `fuel_phase`

Return type `pandas.core.frame.DataFrame`

fuel_radioactivity

Returns the total radioactivity of the solid phase fuel, in units of curies.

Returns `fuel_radioactivity`

Return type `float`

fuel_volume

Returns the total volume of fuel in the entire bucket, in cm^3 .

Returns `fuel_volume`

Return type `float`

gamma_pwr

Returns the amount of gamma radiation given off by the fuel bucket, in units of watts.

Returns `gamma_pwr`

Return type `float`

get_cladding_end_thickness()

Gets the thickness of the hemispherical cladding end caps that are placed on the top and bottom of the fuel slug, in cm.

Returns `cladding_end_thickness`

Return type `float`

get_cladding_mass()

Returns the total mass of cladding material in the bucket, in grams.

Returns `cladding_mass`

Return type `float`

get_cladding_phase()

Returns the phase history of the cladding.

Returns `cladding_phase`

Return type `dataFrame`

get_cladding_volume()

Returns the total volume of cladding in the bucket, in cm^3 .

Returns `cladding_volume`

Return type `float`

get_cladding_wall_thickness()

Returns the thickness of the cladding wall which is on the outside of every fuel slug, and in between both sections of fuel, in cm.

Returns `cladding_wall_thickness`

Return type `float`

`get_fresh_u235_mass()`

Returns the total amount of uranium-235 in the bucket, in grams.

Returns `fresh_u235_mass`

Return type `float`

`get_fresh_u238_mass()`

Returns the total amount of uranium-238 in the bucket, in grams.

Returns `fresh_u238_mass`

Return type `float`

`get_fresh_u_mass()`

Returns the total amount of uranium in the bucket, in grams.

Returns `fresh_u_mass`

Return type `float`

`get_fuel_enrichment()`

Returns the enrichment of the fuel slugs in the bucket, in %.

Returns `fuel_enrichment`

Return type `float`

`get_fuel_mass()`

Returns the total mass of fuel in the solid phase in the bucket.

Returns `fuel_mass`

Return type `float`

`get_fuel_mass_unit()`

Returns the unit that is used to measure the mass of fuel in the bucket.

Returns `fuel_mass_unit`

Return type `str`

`get_fuel_phase()`

Returns the phase history of the fuel.

Returns `fuel_phase`

Return type `pandas.core.frame.DataFrame`

`get_fuel_radioactivity()`

Returns the total radioactivity of the solid phase fuel, in units of curies.

Returns `fuel_radioactivity`

Return type `float`

`get_fuel_volume()`

Returns the total volume of fuel in the entire bucket, in cm^3 .

Returns `fuel_volume`

Return type `float`

get_gamma_pwr()

Returns the amount of gamma radiation given off by the fuel bucket, in units of watts.

Returns gamma_pwr

Return type float

get_heat_pwr()

Returns the total amount of heat generated by the bucket, in units of watts.

Returns heat_pwr

Return type float

get_inner_slug_id()

Returns the inner diameter of the inner section of fuel, in cm.

Returns inner_slug_id

Return type float

get_inner_slug_od()

Returns the outer diameter of the inner section of fuel, in cm.

Returns inner_slug_od

Return type float

get_n_slugs()

Returns the number of fuel slugs in the bucket.

Returns n_slugs

Return type int

get_name()

Returns the name of the fuel bucket.

Returns name

Return type str

get_outer_slug_id()

Returns the inner diameter of the outer section of fuel, in cm.

Returns outer_slug_id

Return type float

get_outer_slug_od()

Returns the outer diameter of the outer section of fuel, in cm. A fuel slug consists of an outer section of fuel and an inner section of fuel, with cladding on the outside of the slug and between the inner and outer sections of fuel.

Returns outer_slug_od

Return type float

get_radioactivity()

Returns the radioactivity of the fuel bucket, in units of curies.

Returns radioactivity

Return type float

get_slug_cladding_volume()

Returns the volume of cladding present in a single fuel slug, in cm³.

Returns slug_cladding_volume

Return type float

get_slug_fuel_volume()

Returns the volume of fuel present in a single fuel slug, in cm³.

Returns slug_fuel_volume

Return type float

get_slug_length()

Returns the length of each slug in the fuel bucket.

Returns slug_length

Return type float

get_slug_type()

Returns the type of slugs being stored in the bucket (inner slug or outer slug).

Returns slug_type

Return type str

heat_pwr

Returns the total amount of heat generated by the bucket, in units of watts.

Returns heat_pwr

Return type float

inner_slug_id

Returns the inner diameter of the inner section of fuel, in cm.

Returns inner_slug_id

Return type float

inner_slug_od

Returns the outer diameter of the inner section of fuel, in cm.

Returns inner_slug_od

Return type float

n_slugs

Returns the number of fuel slugs in the bucket.

Returns n_slugs

Return type int

name

Returns the name of the fuel bucket.

Returns name

Return type str

outer_slug_id

Returns the inner diameter of the outer section of fuel, in cm.

Returns outer_slug_id

Return type float

outer_slug_od

Returns the outer diameter of the outer section of fuel, in cm. A fuel slug consists of an outer section of fuel and an inner section of fuel, with cladding on the outside of the slug and between the inner and outer sections of fuel.

Returns `outer_slug_od`

Return type `float`

radioactivity

Returns the radioactivity of the fuel bucket, in units of curies.

Returns `radioactivity`

Return type `float`

set_cladding_phase (*phase*)

Set's the phase history to specific values.

Parameters `phase` (*dataFrame*) –

set_fuel_phase (*phase*)

Sets the current fuel phase to a specified phase value.

Parameters `phase` (*dataFrame*) –

set_slug_length (*x*)

Sets the length of all slugs in the bucket to x. Used for chopping.

Parameters `x` (*float*) –

slug_cladding_volume

Returns the volume of cladding present in a single fuel slug, in cm^3 .

Returns `slug_cladding_volume`

Return type `float`

slug_fuel_volume

Returns the volume of fuel present in a single fuel slug, in cm^3 .

Returns `slug_fuel_volume`

Return type `float`

slug_length

Returns the length of each slug in the fuel bucket.

Returns `slug_length`

Return type `float`

slug_type

Returns the type of slugs being stored in the bucket (inner slug or outer slug).

Returns `slug_type`

Return type `str`

3.3 fuel_bundle

This FuelBundle class is a container for usage with other plant-level process modules. It is meant to represent a fuel bundle of an oxide fuel LWR reactor. There are three main data structures:

1. fuel bundle specs
2. solid phase
3. gas phase

The container user will have to provide all the data and from then on, this class will help access the data. The printing methods reveal the contained data.

Author: Valmor de Almeida dealmeidav@ornl.gov; vfda Sun Dec 27 15:06:55 EST 2015

class `fuel_bundle.FuelBundle` (*specs=Empty DataFrame Columns: [] Index: []*)

Bases: `object`

fresh_u235_mass

Returns the amount of uranium-235 in the bucket, in grams.

Returns **fresh_u235_mass**

Return type `float`

fresh_u238_mass

Returns the amount of uranium-238 in the bucket, in grams.

Returns **fresh_u238_mass**

Return type `float`

fresh_u_mass

Returns the amount of uranium in the bundle, in grams.

Returns **fresh_u_mass**

Return type `float`

fuel_enrichment

Returns the enrichment of the fuel pins in the bundle, in %.

Returns **fuel_enrichment**

Return type `float`

fuel_mass

Returns the total numerical value for mass of fuel in the solid phase in the bundle.

Returns **fuel_mass**

Return type `float`

fuel_mass_unit

Returns the unit used to measure the mass of fuel in the bundle.

Returns **fuel_mass_unit**

Return type `str`

fuel_pin_length

Returns the length of each fuel pin in the fuel bundle. A fuel pin is a cylindrical section of uranium fuel that is surrounded by cladding.

Returns **fuel_pin_length**

Return type `float`

fuel_pin_radius

Returns the radius of the fuel pin, in cm.

fuel_pin_volume

Returns the volume of fuel in each fuel pin, in cm^3 .

Returns fuel_pin_volume

Return type float

fuel_radioactivity

Returns the total radioactivity of the fuel in the solid phase in the fuel bundle.

Returns fuel_radioactivity

Return type float

fuel_rod_od

Returns the outer diameter of the fuel rod, in cm. A fuel rod consists of a fuel pin surrounded by cladding.

Returns fuel_rod_od

Return type float

fuel_volume

Returns the total volume of fuel in the bundle, in cm^3 .

Returns fuel_volume

Return type float

gamma_pwr

Returns the total amount of gamma radiation given by the fuel bundle, in watts.

Returns gamma_pwr

Return type float

gas_mass

Returns the total numerical value for mass of the fuel in the gas phase.

gas_phase

Returns the gas phase history of the fuel.

Returns gas_phase

Return type dataframe

gas_radioactivity

Returns the total radioactivity of the fuel in the gas phase in the fuel bundle, in curies.

Returns gas_radioactivity

Return type float

get_fresh_U235_mass()

Returns the amount of uranium-235 in the bucket, in grams.

Returns fresh_u235_mass

Return type float

get_fresh_u238_mass()

Returns the amount of uranium-238 in the bucket, in grams.

Returns fresh_u238_mass

Return type float

get_fresh_u_mass()

Returns the amount of uranium in the bundle, in grams.

Returns `fresh_u_mass`

Return type `float`

get_fuel_enrichment()

Returns the enrichment of the fuel pins in the bundle, in %.

Returns `fuel_enrichment`

Return type `float`

get_fuel_mass()

Returns the total numerical value for mass of fuel in the solid phase in the bundle.

Returns `fuel_mass`

Return type `float`

get_fuel_mass_unit()

Returns the unit used to measure the mass of fuel in the bundle.

Returns `fuel_mass_unit`

Return type `str`

get_fuel_pin_length()

Returns the length of each fuel pin in the fuel bundle. A fuel pin is a cylindrical section of uranium fuel that is surrounded by cladding.

Returns `fuel_pin_length`

Return type `float`

get_fuel_pin_radius()

Returns the radius of the fuel pin, in cm.

get_fuel_pin_volume()

Returns the volume of fuel in each fuel pin, in cm³.

Returns `fuel_pin_volume`

Return type `float`

get_fuel_radioactivity()

Returns the total radioactivity of the fuel in the solid phase in the fuel bundle.

Returns `fuel_radioactivity`

Return type `float`

get_fuel_rod_od()

Returns the outer diameter of the fuel rod, in cm. A fuel rod consists of a fuel pin surrounded by cladding.

Returns `fuel_rod_od`

Return type `float`

get_fuel_volume()

Returns the total volume of fuel in the bundle, in cm³.

Returns `fuel_volume`

Return type `float`

get_gamma_pwr()

Returns the total amount of gamma radiation given by the fuel bundle, in watts.

Returns `gamma_pwr`

Return type float

get_gas_mass()

Returns the total numerical value for mass of the fuel in the gas phase.

get_gas_phase()

Returns the gas phase history of the fuel.

Returns gas_phase

Return type dataframe

get_gas_radioactivity()

Returns the total radioactivity of the fuel in the gas phase in the fuel bundle, in curies.

Returns gas_radioactivity

Return type float

get_heat_pwr()

Returns the total amount of heat produced by the fuel bundle, in watts.

Returns heat_pwr

Return type float

get_n_fuel_rods()

Returns the number of fuel rods in the bundle.

Returns n_fuel_rods

Return type int

get_name()

Returns the name of the fuel bundle.

Returns name

Return type str

get_radioactivity()

Returns the total radioactivity of the fuel bundle, in curies.

Returns raduioactivity

Return type float

get_solid_phase()

Returns the solid phase history associated with this fuel bundle.

Returns solidPhase

Return type dataframe

heat_pwr

Returns the total amount of heat produced by the fuel bundle, in watts.

Returns heat_pwr

Return type float

n_fuel_rods

Returns the number of fuel rods in the bundle.

Returns n_fuel_rods

Return type int

name
Returns the name of the fuel bundle.

Returns name
Return type `str`

radioactivity
Returns the total radioactivity of the fuel bundle, in curies.

Returns raduioactivity
Return type `float`

set_fuel_pin_length(*x*)
Sets the length of all fuel pins in the bundle to *x*.

Returns x
Return type `float`

set_gas_phase(*phase*)
Sets the gas phase history of the fuel equal to *phase*.

Parameters phase (*dataFrame*) –

set_solid_phase(*phase*)
Sets the solid phase history of the fuel equal to *phase*.

Parameters phase (*dataFrame*) –

solid_phase
Returns the solid phase history associated with this fuel bundle.

Returns solidPhase
Return type `dataFrame`

3.4 fuel_segment

Fuel segment Author: Valmor de Almeida dealmeidav@ornl.gov; vfda Sat Jun 27 14:46:49 EDT 2015

class `fuel_segment.FuelSegment` (*geometry=Series([], dtype: float64), species=[]*)
Bases: `object`

__repr__()
Used to pront the geometry of the fuel segment and the species that it consists of.

Returns s
Return type `str`

__str__()
Used to print the geometry of the fuel segment and the species that it consists of.

Returns s
Return type `str`

geometry
Returns the geometry of the fuel bundle (cylindrical, hexoganol, rectangular, etc).

Returns geometry
Return type `str`

get_attribute (*name*, *nuclide=None*, *series=None*)

Used to get stored fuel segment properties, either overall (as an average), or on a nuclide basis. “name” in this case refers to the attribute in question. At this point in time, series is not implemented and passing it to this function will result in an error. Possible attributes that may be retrieved with this function, as well as the name to pass to this function to retrieve them are: number of segments in the bundle (n-segments, always equal to 1), the id of the segment that makes up the bundle (segment-id), the volume of the fuel in the bundle (fuel-volume), the total volume of the segment (segment-volume), the diameter (fuel-diameter) and length (fuel-length) of the segment, the mass or mass density of the segment (mass or mass-cc, respectively), or the total or per-volume radioactivity, gamma radiation density or heat density of the fuel segment (radioactivity and radioactivityDens, gamma and gamma-dens, and heat and heat-dens, respectively).

Finally, density or total mass of a specific nuclide can be determined by passing a specific nuclide to the function, with a name value of mass or mass-cc.

Parameters

- **name** (*str*) –
- **nuclide** (*str*) –

Returns

Return type many types

get_geometry ()

Returns the geometry of the fuel bundle (cylindrical, hexagonal, rectangular, etc).

Returns geometry

Return type *str*

get_specie (*name*)

Returns a specie named [name] from the list of species making up the fuel bundle. If no name is specified, this function will return None.

Parameters **name** (*str*) –

Returns specie

Return type *obj*

get_species ()

Returns the species object which describes the composition of the fuel bundle. The species encapsulates all chemical species present in the fuel bundle.

Returns species

Return type *object*

specie

Returns a specie named [name] from the list of species making up the fuel bundle. If no name is specified, this function will return None.

Parameters **name** (*str*) –

Returns specie

Return type *obj*

species

Returns the species object which describes the composition of the fuel bundle. The species encapsulates all chemical species present in the fuel bundle.

Returns species

Return type `object`

3.5 fuelsegmentsgroups

Author: Valmor de Almeida dealmeidav@ornl.gov; vfda

Fuel segment

VFdALib support classes

Sat Jun 27 14:46:49 EDT 2015

class `fuelsegmentsgroups.FuelSegmentsGroups` (*key=None, fuelSegments=None*)

Bases: `object`

Creates a dictionary of lists of fuel segment objects, with the keys typically being timestamps. Each fuel segment object has two data members, a *Pandas* Series for geometry spec and a *panda* DataFrame for property density.

AddGroup (*key, fuelSegments=None*)

Appends the dictionary with a new key and associated list of fuelSegments. If the specified key is already present in the dictionary, then the specified list of fuel segments will be appended to the list of fuel segments already associated with the specified key.

Parameters

- **key** (*str*) –
- **fuelSegments** (*list*) –

GetAttribute (*groupKey=None, attributeName=None, nuclideSymbol=None, nuclideSeries=None*)

Returns the average value of an attribute amongst all elements in a group (WARNING: keys with no values associated with them will lower this average!). If *groupKey* is not specified, the function will return the average attribute value of every fuel segment element in the entire dictionary. If *attribute* is not specified, the function call will fail. If the key value specified does not match any keys in the dictionary, the function will return a value of 0.

Parameters

- **groupKey** (*str*) –
- **attributeName** (*str*) –
- **nuclideSymbol** (*str*) –
- **nuclideSeries** (*str*) –

Returns `groupAttribute`

Return type `float`

GetFuelSegments (*groupKey=None*)

Returns a list of fuel segments associated with a specified groupkey. If no group key is specified, then all elements in the dictionary will be returned. If the specified group key does not exist, then the function will return an empty list.

Parameters **groupKey** (*str*) –

Returns `fuelSegments`

Return type `list`

HasGroup (*key*)

Checks if the specified key has a group of fuel segments associated with it.

Parameters `key` (*str*) –

Returns `key`

Return type `str`

RemoveFuelSegment (*groupKey*, *fuelSegment*)

Removes a fuel segment from a list associated with a specified group key. If the specified group key or fuel segment do not exist, the function will fail.

Parameters

- **groupKey** (*str*) –
- **fuelSegment** (*str*) –

Returns

Return type `empty`

3.6 fuelslug

Author: Valmor de Almeida dealmeidav@ornl.gov; vfda

Fuel slug

3.6.1 ATTENTION:

This container requires two Phase() containers which are by definition histories. The history is not checked. Therefore any inconsistency will be propagated forward. A fuel slug has two solid phases: cladding and fuel. The user will decide how to best use the underlying history data in the Phase() container of each phase.

VFdALib support classes

Thu Dec 15 16:18:39 EST 2016

```
class fuelslug.FuelSlug(specs=Series([], dtype: float64), fuelPhase= **Phase(): time unit: s *quantities*: None *species*: None *history* #time_stamp=1 *history end* @0.0 Series([], Name: 0.0, dtype: float64), claddingPhase= **Phase(): time unit: s *quantities*: None *species*: None *history* #time_stamp=1 *history end* @0.0 Series([], Name: 0.0, dtype: float64))
```

Bases: `object`

GetAttribute (*name*, *phase=None*, *symbol=None*, *series=None*)

Returns the value of the specified attribute. Any attribute that is specified in class construction can be retrieved using this function. The attribute may also be retrived from a speciefic phase, a specific nuclide OR a specific series.

Parameters

- **name** (*str*) –
- **phase** (*str*) –
- **symbol** (*str*) –
- **series** (*str*) –

Returns `attribute`

Return type `int` or `float`

GetCladdingPhase ()

Returns the phase history of the cladding.

Returns `claddingPhase`

Return type `dataFrame`

GetFuelPhase ()

Returns the phase history of the solid fuel.

Returns `fuelPhase`

Return type `dataFrame`

GetSpecs ()

Returns the species associated with this fuel slug.

Returns `specs`

Return type `str`

ReduceCladdingVolume (*dissolvedVolume*)

Reduces the amount of cladding in the slug by dissolvedvolume. This will also update the dimensions of the cladding walls and end caps; volume will be taken from all sections equally such that the relative dimensions stay the same.

Parameters `dissolvedVolume (float)` –

ReduceFuelVolume (*dissolvedVolume*)

Reduces the amount of fuel in the slug by dissolvedVolume. This will also update the dimensions of the fuel slug, mainly the thickness of each fuel layers.

Parameters `dissolvedVolume (float)` –

claddingPhase

Returns the phase history of the cladding.

Returns `claddingPhase`

Return type `dataFrame`

fuelPhase

Returns the phase history of the solid fuel.

Returns `fuelPhase`

Return type `dataFrame`

specs

Returns the species associated with this fuel slug.

Returns `specs`

Return type `str`

3.7 nuclides

Author: Valmor de Almeida dealmeidav@ornl.gov; vfda

Nuclides container. The purpose of the this container is to store and query a table of nuclides. Typically the table is filled in with data from an ORIGEN calculation or some other fission/transmutation code.

VFdALib support classes

Sat Jun 27 14:46:49 EDT 2015

```
class nuclides.Nuclides (propertyDensities=Empty DataFrame Columns: [] Index: [])
    Bases: object

    GetAttribute (name, symbol=None, series=None)
```

3.8 periodictable

Properties of the chemical elements.

Each chemical element is represented as an object instance. Physicochemical and descriptive properties of the elements are stored as instance attributes.

Author Christoph Gohlke

Version 2015.01.29

Radiochemical data (isotopes) has been added to this table (2015-2016) Origin: <http://www.radiochemistry.org/> Valmor F. de Almeida: dealmeidavf@gmail.com; dealmeidav@ornl.gov

3.8.1 Requirements

- CPython 2.7 or 3.4

References

1. <http://physics.nist.gov/PhysRefData/Compositions/>
2. <http://physics.nist.gov/PhysRefData/IonEnergy/tblNew.html>
3. [http://en.wikipedia.org/wiki/%\(element.name\)s](http://en.wikipedia.org/wiki/%(element.name)s)
4. <http://www.miranda.org/~jkominek/elements/elements.db>

Examples

```
>>> from elements import ELEMENTS
>>> len(ELEMENTS)
109
>>> str(ELEMENTS[109])
'Meitnerium'
>>> ele = ELEMENTS['C']
>>> ele.number, ele.symbol, ele.name, ele.eleconfig
(6, 'C', 'Carbon', '[He] 2s2 2p2')
>>> ele.eleconfig_dict
{(1, 's'): 2, (2, 'p'): 2, (2, 's'): 2}
>>> sum(ele.mass for ele in ELEMENTS)
14659.1115599
>>> for ele in ELEMENTS:
...     ele.validate()
...     ele = eval(repr(ele))
```

3.9 phase

Phase *history* container. When you think of a phase value, think of that value at a specific point in time. This container holds the historic data of a phase; its species and quantities. This implementation treats access of time stamps within a tolerance. All searches for time stamped values are subjected to an approximation of the time stamp to avoid storing values too close to each other in time, and/or to return the closest value in time searched or no value if none can be found according to the tolerance.

3.9.1 Background

TODO: ATTENTION: The species (list of *Specie*) AND quantities (list of *Quantity*) data members have ARBITRARY density values either at an arbitrary point in the history or at no point in the history. This needs to be removed in the future to avoid confusion.

To obtain history values, associated to the phase, at a particular point in time, use the `GetValue()` method to access the history data frame (pandas) via columns and rows. ALERT: The corresponding values in species and quantities are OVERRIDEN and NOT to be used through the phase interface.

Author: Valmor F. de Almeida dealmeidav@ornl.gov; vfda Sat Sep 5 01:26:53 EDT 2015

Cortix: a program for system-level modules coupling, execution, and analysis.

class `phase.Phase` (*time_stamp=None, time_unit=None, species=None, quantities=None*)

Bases: `object`

Phase *history* container. A *Phase* consists of *Species* and *Quantities* varying with time. This container is meant to reproduce the basic idea of a material phase.

AddQuantity (*newQuant*)

Adds a new quantity object to the dataframe. See `quantity.py` for more details on the quantity class.

Parameters *newQuant* (`object`) –

AddRow (*try_time_stamp, row_values*)

Adds a row to the dataframe, with a timestamp of *try_time_stamp* and row values equal to *row_values*. Take care that the dimensions and order of the data matches up!

Parameters

- *try_time_stamp* (`float`) –
- *row_values* (`list`) –

AddSpecie (*new_specie*)

Adds a new specie object to the phase history. See `species.py` for more details on the specie class.

Parameters *new_specie* (`obj`) –

ClearHistory (*value=0.0*)

Set species and quantities of history to a given value (default to zero value), all time stamps are preserved.

Parameters *value* (`float`) –

GetActors ()

Returns a list of all the actors in the phase history.

Returns `list(self.__phase.columns)`

Return type `list`

GetColumn (*actor*)

Returns an entire column of data. A column is the entire history of data associated with a specific actor.

Parameters `actor (str)` –

Returns `list(self.__phase.loc[`

Return type `, actor])`: list

GetQuantities ()

Returns the list of *Quantities*. The values in each *Quantity* are synchronized with the *Phase* data frame.

Returns quantities

Return type list

GetQuantity (*name*)

Returns the quantity evaluated at the last time step of the phase history. This also updates the value of the quantity object. If the quantity name does not exist the return is None.

Parameters `name (str)` –

GetRow (*try_time_stamp=None*)

Returns an entire row of the phase dataframe. A row is a series of values that are all at the same time stamp.

Parameters `try_time_stamp (float)` –

Returns `list(self.__phase.loc[time_stamp,`

Return type `])`: list

GetSpecie (*name*)

Returns the species specified by name if it exists, or none if it doesn't.

Parameters `name (str)` –

Returns specie

Return type str

GetSpecies ()

Returns every single species in the phase history.

Returns species

Return type list

GetTimeStamps ()

Returns a list of all the time stamps in the phase history.

Returns timeStamps

Return type list

GetValue (*actor, try_time_stamp=None*)

Deprecated: use `get_value()`

ResetHistory (*try_time_stamp=None, value=None*)

Set species and quantities of history to a given value (default to zero value) only one time stamp is preserved (default to last time stamp).

Parameters

- `try_time_stamp (float)` –

- `value (float)` –

ScaleRow (*try_time_stamp, value*)

Multiplies all of the data in a row (except time stamp) by a scalar value.

Parameters

- **try_time_stamp** (*float*) –
- **value** (*float*) –

SetSpecieId (*name*, *val*)

Sets the flag of a specie “name” equal to val.

Parameters

- **name** (*str*) –
- **val** (*int*) –

SetValue (*actor*, *value*, *try_time_stamp=None*)

For the record: old def SetValue(self, time_stamp, actor, value):

Parameters

- **actor** (*str*) –
- **value** (*float*) –
- **try_time_stamp** (*float*) –

WriteHTML (*fileName*)

Convert the *Phase* container into an HTML file.

Parameters **fileName** (*str*) –

__init__ (*time_stamp=None*, *time_unit=None*, *species=None*, *quantities=None*)

Sometimes an empty *Phase* object is created by user code. This case needs adequate logic for *None* types. Note on usage: when passing quantities, do set the value argument explicitly to help define the type and avoid SetValue() errors with Pandas. This is to be investigated later. Also, the usage of a *DataFrame* needs to be re-evaluated. Maybe better to use a *Quantity* object and a *Specie* object with a *Pandas Series* history as a value to avoid the existence of a value in *Quantity* and a value in *Phase* that are not in sync.

get_quantity (*name*, *try_time_stamp=None*)

New version. Get the quantity *name* at a point in time closest to *try_time_stamp* up to a tolerance. If no time stamp is passed, the whole history is returned.

Parameters

- **name** (*str*) –
- **try_time_stamp** (*float*, *int* or *None*) – Time stamp of desired quantity value.
Default: *None* returns the whole quantity history.

Returns *quant.value*

Return type *float* or *int* or other

get_quantity_history (*name*)

Create a *Quantity name* history. This will create a fully qualified *Quantity* object and return to the caller. The function is typically needed for data output to a file through *pickle*. Since the value attribute of a quantity can be any data structure, a time-series is built on the fly and stored in the value attribute. In addition the time unit is added to the final return value as a tuple.

Parameters **name** (*str*) –

Returns *quant_history*

Return type *tuple(Quantity, str)*

get_value (*actor*, *try_time_stamp=None*)

Returns the value associated with a specified actor at a specified time stamp.

Parameters

- **actor** (*str*) –
- **try_time_stamp** (*float*) –

Returns `self.__phase.loc[time_stamp, actor]`

Return type `float`

has_time_stamp (*try_time_stamp*)

Checks to see if `try_time_stamp` exists in the phase history.

Parameters `try_time_stamp` –

quantities

Returns the list of *Quantities*. The values in each *Quantity* are synchronized with the *Phase* data frame.

Returns `quantities`

Return type `list`

set_value (*actor*, *value*, *try_time_stamp=None*)

New version. Discontinue using `SetValue()`

species

Returns every single species in the phase history.

Returns `species`

Return type `list`

timeStamps

Returns a list of all the time stamps in the phase history.

Returns `timeStamps`

Return type `list`

time_stamps

Get all time stamps in the index of the data frame.

Returns `time_stamps`

Return type `list`

time_unit

Returns the time unit of the *Phase*.

Returns `time_unit`

Return type `str`

3.10 quantity

Author: Valmor de Almeida dealmeidav@ornl.gov; vfda

This Quantity class is to be used with other classes in plant-level process modules.

For unit testing do at the linux command prompt: `python quantity.py`

Sat Sep 5 12:51:34 EDT 2015

```
class quantity.Quantity(name='null-quantity', formalName='null-quantity', value=0.0,  
                        unit='null-unit')
```

Bases: `object`

todo: this probably should not have a “value” for the same reason as `Specie`. this needs some thinking.

well not so fast. This can be used to build a quantity with anything as a value. For instance a history of the quantity as a time series.

GetFormalName()

Returns the formal name of the quantity.

Returns `formalName`

Return type `str`

GetUnit()

Returns the units of the quantity.

Returns `unit`

Return type `str`

GetValue()

Gets the numerical value of the quantity.

Returns `value`

Return type any type

SetFormalName(fn)

Sets the formal name of the property to fn.

Parameters `fn(str)` –

SetName(n)

Sets the name of the quantity in question to n.

Parameters `n(str)` –

SetUnit(f)

Sets the units of the quantity to f (for example, density would be in units of g/cc.

Parameters `f(str)` –

SetValue(v)

Sets the numerical value of the quantity to v.

Parameters `v(float)` –

__repr__()

Used to print the data stored by the quantity class. Will print out name, formal name, the value of the quantity and its unit.

Returns `s`

Return type `str`

__str__()

Used to print the data stored by the quantity class. Will print out name, formal name, the value of the quantity and its unit.

Returns `s`

Return type `str`

formalName

Returns the formal name of the quantity.

Returns formalName

Return type str

formal_name

Returns the formal name of the quantity.

Returns formalName

Return type str

get_name()

Returns the name of the quantity.

Returns name

Return type str

name

Returns the name of the quantity.

Returns name

Return type str

plot (*x_scaling=1, y_scaling=1, title=None, x_label='x', y_label=None, file_name=None, same_axis=True, dpi=300*)

This will support a few possibilities for data storage in the self.__value member.

Pandas Series. If self.__value is a Pandas Series, plot against the index. However the type stored in the Series matter. Suppose it is a series of a *numpy* array. This must be of the same rank for every entry. This plot method assumes it is an iterable type of the same length for every entry in the series. A plot of all elements in the type against the index of the series will be made. The plot may have all elements in one axis or each element in its own axis.

unit

Returns the units of the quantity.

Returns unit

Return type str

value

Gets the numerical value of the quantity.

Returns value

Return type any type

3.11 specie

Author: Valmor de Almeida dealmeidav@ornl.gov; vfda

This Specie class is to be used with other classes in plant-level process modules.

NB: Species is always used either in singular or plural cases, the class named here reflects one species. If many species are used in an external context, the species object name can be used without conflict.

For unit testing do at the linux command prompt: python specie.py

NB: The `Specie()` class encapsulates either the molecular or empirical chemical formula of a compound. This is done as follows. Say MAO2 is either a molecular or empirical chemical formula of a fictitious compound denoting minor actinides dioxide. The list of atoms is given as follows:

```
['0.49*Np-237', '0.42*Am-241', '0.08*Am-243', '0.01*Cm-244', '2.0*O-16']
```

note the MA forming nuclides add to 1 = 0.49 + 0.42 + 0.08 + 0.01. Therefore the number of atoms in this compound is 3. 1 MA “atom” and 2 O. Note that the total number of “atoms” is obtained by summing all multipliers: 0.49 + 0.42 + 0.08 + 0.01 + 2.0. The nuclide is indicated by the element symbol followed by a dash and the atomic mass number. Here the number of nuclide types is 5 (`self._nNuclideTypes`).

The numbers preceeding the nuclide symbol before the * will be referred to as multipliers. The sum of the multipliers will add to the number of “atoms” in the formula. **WARNING:** a multiplier could be in the format 0.00e-00. In this case a hiphen may appear twice, e.g.: 1.549e-09*U-233

Other forms can be used for common true species

```
['Np-237', '2.0*O-16'] or ['Np-237', 'O-16', 'O-16'] or [ '2*H', 'O' ] or [ 'H', 'O', 'H' ] etc...
```

This code will calculate the molar mass of any species with a given valid atom list using a provided periodic table of chemical elements. The user can also reset the value of the molar mass with a setter method.

Sat May 9 21:40:48 EDT 2015 created; vfda

```
class specie.Specie (name='null', formula_name='null', phase='null', atoms=[], molarCC=0.0,
                      massCC=0.0, flag=None)
```

Bases: `object`

todo: phase should not be here; concentrations should not be here only molar quantities should be here see the Phase container

GetAtoms ()

GetFlag ()

Returns the flag associated with the species.

Returns flag

Return type `str`

GetFormula ()

Returns the molecular or empirical formula of the species. It is usually a list, for example, of the form ['2*H', 'O'].

Returns formula

Return type `list`

GetFormulaName ()

Returns the formulaic name of the compound. For example, “Dihydrogen monoxide”.

Returns self.__formula_name

Return type `str`

GetMassCC ()

Returns the numerical value of the mass density of the species (mass/volume).

Returns massCC

Return type `float`

GetMassCCUnit ()

Returns the unit used to measure the mass density of the species.

Returns massCCUnit

Return type `str`

GetMolarCC ()

Returns the numerical value for the number (molar) density of the species (moles/volume).

Returns `molarCC`

Return type `float`

GetMolarCCUnit ()

Returns the unit used to measure molar density of the species.

Returns `molarCCUnit`

Return type `str`

GetMolarGammaPwr ()

Returns the amount of gamma radiation produced per mole of this species (measured in units of power).

Returns `molarGammaPwr`

Return type `float`

GetMolarGammaPwrUnit ()

Returns the unit used to measure the amount of gamma radiation produced per mole of this species.

Returns `molarGammaPwrUnit`

Return type `str`

GetMolarHeatPwr ()

Returns the amount of heat generated per mole of this species.

Returns `molarHeatPwr`

Return type `float`

GetMolarHeatPwrUnit ()

Returns the unit used to measure the amount of heat generated per mole of this species.

Returns `molarHeatPwrUnit`

Return type `str`

GetMolarMass ()

Returns the numerical value for the molar mass of the species. Units are given by `molarMassUnit`.

Returns `molarMass`

Return type `float`

GetMolarMassUnit ()

Returns the unit used to measure the molar mass of the species.

Returns `molarMassUnit`

Return type `str`

GetMolarRadioactivity ()

Returns the numerical value for molar radioactivity of the species.

Returns `molarRadioactivity`

Return type `float`

GetMolarRadioactivityFractions ()

Returns a list of numbers that specifies the % of molar reactivity that comes from each type of atom in the

species. For example, a `molarRadioactivityFraction` of `[0.65, 0.35]` for water means that 65% of the molar radioactivity comes from the hydrogen atoms and 35% comes from the oxygen atom.

Returns `molarRadioactivityFractions`

Return type `list`

GetMolarRadioactivityUnit ()

Returns the unit used to measure molar radioactivity.

Returns `molarRadioactivityUnit`

Return type `str`

GetNAtoms ()

Returns the total number of atoms comprising the species. For example, water is comprised of three atoms.

Returns `nAtoms`

Return type `int`

GetNNuclideTypes ()

Returns the number of different types of atoms comprising the species. For example, water is composed of two different types of atoms, hydrogen and oxygen.

Returns `nNuclideTypes`

Return type `int`

GetName ()

Returns the empirical name of the species. For example, “water”.

Returns `name`

Return type `str`

GetPhase ()

Returns the phase history of the species.

Returns `phase`

Return type `dataFrame`

SetAtoms (*atoms*)

SetFlag (*f*)

Sets the flag associated with the species to *f*.

Parameters *f* (`str`) –

SetFormula (*atoms*)

Sets the species’ formula equal to *atoms*. Will automatically update the molar mass of the species, and will also fail if *atoms* is not a list of strings.

Parameters *atoms* (`list`) –

SetFormulaName (*f*)

Sets the formulaic name to *f*.

Returns `self.__formula_name`

Return type `str`

SetMassCC (*v*)

Sets the numerical value of the mass density equal to *v*.

Parameters *v* (`float`) –

SetMassCCUnit (*v*)

Sets the units used to measure mass density to *v*.

Parameters *v* (*str*) –

SetMolarCC (*v*)

Sets the numerical value for the molar density of the species to *v*.

Parameters *v* (*float*) –

SetMolarCCUnit (*v*)

Sets the unit used to measure the molar density of the species to *v*.

Parameters *v* (*str*) –

SetMolarGammaPwr (*v*)

Sets the amount of gamma radiation produced per mole of this species to *v*.

Parameters *v* (*float*) –

SetMolarGammaPwrUnit (*v*)

Sets the unit used to measure the amount of gamma radiation produced per mole of this species to *v*.

Parameters *v* (*str*) –

SetMolarHeatPwr (*v*)

Sets the amount of heat generated per mole of this species to *v*.

Parameters *v* (*float*) –

SetMolarHeatPwrUnit (*v*)

Sets the unit used to measure the amount of heat generated per mole of this species to *v*.

Parameters *v* (*str*) –

SetMolarMass (*v*)

Sets the molar mass of the species equal to *v*.

Parameters *v* (*float*) –

SetMolarMassUnit (*v*)

Sets the unit used to measure the molar mass of the species to *v*.

Parameters *v* (*str*) –

SetMolarRadioactivity (*v*)

Sets the molar radioactivity of the species equal to *v*.

Parameters *v* (*float*) –

SetMolarRadioactivityFractions (*fracs*)

Sets molarRadioactivityFractions equal to *fracs*. *Fracs* must be a list of floats with the same length as there are different atoms in the species, or the function call will fail. (e.g. `self._atoms` and *fracs* must be of the same length). Take care to ensure that the elements of *fracs* match with the elements of `self._atoms`! (65% is in the same position in *fracs* as hydrogen is in `self._atoms`, following the above example).

Parameters *fracs* (*list*) –

SetMolarRadioactivityUnit (*v*)

Sets the unit used to measure molar radioactivity to *v*.

Parameters *v* (*str*) –

SetName (*n*)

Sets the empirical name of the species to *n*.

Parameters `n` (*str*) –

SetPhase (*p*)

Sets the phase history to *p*.

Parameters `p` (*dataFrame*) –

atoms

flag

Returns the flag associated with the species.

Returns `flag`

Return type `str`

formula

Returns the molecular or empirical formula of the species. It is usually a list, for example, of the form ['2*H', 'O'].

Returns `formula`

Return type `list`

formula_name

Returns the formulaic name of the compound. For example, "Dihydrogen monoxide".

Returns `self.__formula_name`

Return type `str`

massCC

Returns the numerical value of the mass density of the species (mass/volume).

Returns `massCC`

Return type `float`

massCCUnit

Returns the unit used to measure the mass density of the species.

Returns `massCCUnit`

Return type `str`

molarCC

Returns the numerical value for the number (molar) density of the species (moles/volume).

Returns `molarCC`

Return type `float`

molarCCUnit

Returns the unit used to measure molar density of the species.

Returns `molarCCUnit`

Return type `str`

molarGammaPwr

Returns the amount of gamma radiation produced per mole of this species (measured in units of power).

Returns `molarGammaPwr`

Return type `float`

molarGammaPwrUnit

Returns the unit used to measure the amount of gamma radiation produced per mole of this species.

Returns `molarGammaPwrUnit`

Return type `str`

molarHeatPwr

Returns the amount of heat generated per mole of this species.

Returns `molarHeatPwr`

Return type `float`

molarHeatPwrUnit

Returns the unit used to measure the amount of heat generated per mole of this species.

Returns `molarHeatPwrUnit`

Return type `str`

molarMass

Returns the numerical value for the molar mass of the species. Units are given by `molarMassUnit`.

Returns `molarMass`

Return type `float`

molarMassUnit

Returns the unit used to measure the molar mass of the species.

Returns `molarMassUnit`

Return type `str`

molarRadioactivity

Returns the numerical value for molar radioactivity of the species.

Returns `molarRadioactivity`

Return type `float`

molarRadioactivityFractions

Returns a list of numbers that specifies the % of molar reactivity that comes from each type of atom in the species. For example, a `molarRadioactivityFraction` of [0.65, 0.35] for water means that 65% of the molar radioactivity comes from the hydrogen atoms and 35% comes from the oxygen atom.

Returns `molarRadioactivityFractions`

Return type `list`

molarRadioactivityUnit

Returns the unit used to measure molar radioactivity.

Returns `molarRadioactivityUnit`

Return type `str`

nAtoms

Returns the total number of atoms comprising the species. For example, water is comprised of three atoms.

Returns `nAtoms`

Return type `int`

nNuclideTypes

Returns the number of different types of atoms comprising the species. For example, water is composed of two different types of atoms, hydrogen and oxygen.

Returns `nNuclideTypes`

Return type `int`

name

Returns the empirical name of the species. For example, “water”.

Returns `name`

Return type `str`

phase

Returns the phase history of the species.

Returns `phase`

Return type `dataFrame`

3.12 stream

Author: Valmor F. de Almeida dealmeidav@ornl.gov; vfda

Stream container

VFdALib support classes

Sat Aug 15 17:24:02 EDT 2015

class `stream.Stream` (*timeStamp*, *species=None*, *quantities=None*, *values=0.0*)

Bases: `object`

GetActors ()

Returns the actors present in the stream of data.

Returns `list(self.stream.columns)`

Return type `list`

GetQuantities ()

Returns all the quantities given by the stream.

Returns `self.quantities`

Return type `list`

GetQuantity (*name*)

Returns the specified quantity called “name” from the stream, or none if the specified name does not exist.

Parameters `name` (*str*) –

Returns `quant`

Return type `float`

GetRow (*timeStamp=None*)

Returns an entire row of data from the stream. A row of data is all the data in a dataframe at a specified time stamp, given by *timeStamp*. If *timeStamp* is not specified, this function will return the entire stream dataframe.

Parameters `timeStamp` (*float*) –

Returns

- `self.stream.loc[self.timestamp, ()]` or `self.stream.loc[timeStamp, :]`
- `list`

GetSpecie (*name*)

Returns a specie named “name” from the stream.

Parameters **name** (*str*) –

Returns **specie**

Return type **obj**

GetSpecies ()

Returns a list of all species in the stream.

Returns **self.species**

Return type **list**

GetTimeStamp ()

Returns the time stamp of the stream.

Returns **self.timeStamp**

Return type **float**

GetValue (*actor, timeStamp=None*)

Returns the value associated with a specified “actor” at a specified “timeStamp”. If no timeStamp is specified, then the function will return all values associated with the specified actor at all time stamps.

Parameters

- **actor** (*str*) –
- **timeStamp** (*float*) –

Returns

- *self.stream.loc[self.timeStamp, actor] or self.stream.loc[timeStamp,*
- *actor]* (*list or float, respectively.*)

SetSpecieId (*name, val*)

Sets the numerical id of the specie of name “name” to val.

Parameters

- **name** (*str*) –
- **val** (*int*) –

SetValue (*actor, value=None, timeStamp=None*)

Sets the value associated with a specified actor at a specified timeStamp to “value”. If no value is specified, the value will default to 0.0. If no timeStamp is specified, it will set all values associated with actor to the specified value (or 0.0 if value = None).

Parameters

- **actor** (*str*) –
- **value** (*float*) –
- **timeStamp** (*float*) –

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