Cortix Documentation

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CHAPTER

ONE

SRC

1.1 cortix_main

```
Bases: object
Cortix main class definition.
The typical Cortix run file workflow:
  1. Create the Cortix object
  2. Add and connect Modules
  3. Run and close Cortix
use mpi
     bool - True for MPI, False for Multiprocessing.
use_multiprocessing
     bool - False for MPI, True 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.
```

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

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 Cortix Simulation

Parameters m (Module) - The Module object to be added

close()

Closes the cortix object properly before destruction.

User is advised to call this method at the end of the run file.

```
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 Cortix 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 Cortix 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 Cortix simulation.

This function concurrently executes the *cortix.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

Cortix module super class.

This class provides facilities for creating modules within the Cortix network. Cortix 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 Cortix 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*.

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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

use_multiprocessing

bool - False for MPI, True for Multiprocessing

ports

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

```
__init__()
```

Module super class constructor.

Note: 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 either their ports directly or inferred ports.

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 corresponding 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

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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 self.use_multiprocessing:

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

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

Warning: This function must be overridden by all Cortix modules

Parameters

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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 \\ \mathbf{name} \\ string
```

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```
use_mpi
     bool
\underline{\hspace{0.1cm}}eq\underline{\hspace{0.1cm}} (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

```
\mathtt{send}\left(data, tag=None\right)
```

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

1.3. port module 5

CHAPTER

TWO

EXAMPLES

2.1 adjudication module

```
class adjudication.Adjudication(n_groups=1, pool_size=0.0)
    Bases: cortix.src.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 overriden 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 self.use_multiprocessing:

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

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

Warning: This function must be overridden by all Cortix modules

Parameters

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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 overriden 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 self.use multiprocessing:

```
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.
```

2.2. arrested module 7

Warning: This function must be overridden by all Cortix modules

Parameters

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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

Community Cortix 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 overriden 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 self.use_multiprocessing:

```
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

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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 overriden 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 self.use_multiprocessing:

```
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

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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 overriden 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 self.use_multiprocessing:

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

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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: 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 overriden 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 self.use_multiprocessing:

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

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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 overriden 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 self.use_multiprocessing:

```
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

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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.

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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 overriden 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 self.use_multiprocessing:

```
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

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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
```

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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 self.use_multiprocessing:

```
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

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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

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 self.use_multiprocessing:

```
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

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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: cortix.src.module.Module
```

Probation Cortix 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

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 self.use_multiprocessing:

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

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

Warning: This function must be overridden by all Cortix modules

Parameters

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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. It 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 \ vortex + 1 \ 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
run_droplet_a.main()
    Cortix run file for a Droplet-Vortex network.
    run_droplet_a.n_droplets
        int - Number of droplets to use (one per process).
    run_droplet_a.end_time
        float - End of the flow time in SI unit.
```

```
run_droplet_a.time_step
    float - Size of the time step between port communications in SI unit.

run_droplet_a.create_plots
    bool - Create various plots and save to files. (all data collected in the parent process; it may run out of memory).

run_droplet_a.plot_vortex_profile
    bool - Whether to plot (to a file) the vortex function used.

run_droplet_a.use_mpi
    bool - If set to True use MPI otherwise use Python multiprocessing.
```

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 \ vortex + 1 \ data\_plot + 1 \ 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 \ vortex + 1 \ 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 network dynamics modeling.

This example uses 7 modules:

- Community
- · Arrested
- Adjudication
- Jail
- Prison
- Probation
- Parole

and a population balance model is used to follow the offenders population groups between modules.

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

```
nprocs = 7 + 1 cortix
```

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

```
mpiexec -n nprocs run_justice.py
```

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

```
run_justice.py
run_justice.main()
    Cortix run file for a criminal justice network.

run_justice.n_groups
    int - Number of population groups being followed. This must be the same for all modules.

run_justice.end_time
    float - End of the flow time in SI unit.

run_justice.time_step
    float - Size of the time step between port communications in SI unit.

run_justice.use_mpi
```

bool - If set to True use MPI otherwise use Python multiprocessing.

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
```

2.15. vortex module

```
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 overriden 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 self.use_multiprocessing:

```
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

- arg[0] (int) Index of the state in the communication queue.
- arg[1] (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.

2.15. vortex module

CHAPTER

THREE

SUPPORT

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 Cortix 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

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 cm³.

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

${\tt fresh_u_mass}$

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 cm³.

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 cm³.

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<sup>3</sup>.
         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
```

3.2. fuel bucket 24

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

get slug cladding volume()

```
Returns slug_cladding_volume
         Return type float
get_slug_fuel_volume()
     Returns the volume of fuel present in a single fuel slug, in cm<sup>3</sup>.
         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 cm³.

Returns slug_cladding_volume

Return type float

slug_fuel_volume

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

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 acess 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 cylindircal 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 cm³.

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 cm³.

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 cylindircal 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 cm<sup>3</sup>.
         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()
```

3.3. fuel bundle 29

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

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

Returns fuel volume

Returns gamma pwr

Return type float

get_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

3.4. fuel segment 31

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, hexoganol, 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

3.4. fuel segment 32

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

```
\textbf{class} \ \texttt{fuelsegmentsGroups}. \textbf{\textit{FuelSegmentsGroups}} \ (\textit{\textit{key=None}}, \textit{\textit{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(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 retrieved from a specific phase, a specific nuclide OR a specific series.

Parameters

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

Returns attribute

Return type int or float

3.6. fuelslug 34

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

3.7. nuclides 35

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
- 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))
```

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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 by 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.colums)
```

Return type list

GetColumn (actor)

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

3.9. phase 37

```
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.

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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 existance 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)

3.9. phase 39

```
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

3.10. quantity 40

```
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
```

3.10. quantity 41

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

This will support a few possibities 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 ficticious 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 preceding 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

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 speciefies 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) -
```

${\tt SetFormulaName}\,(f)$

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) -

${\tt SetMolarGammaPwrUnit}\;(v)$

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

Parameters $\mathbf{v}(str)$ –

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 floatswith 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) –

${\tt SetName}\ (n)$

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 speciefies 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

 ${\tt GetRow}~(timeStamp{=}None)$

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

3.12. stream 49

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) -

${\tt SetValue}\:(actor, value = None, timeStamp = None)$

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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