
Cortix Documentation

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1.1 cortix_main

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

Bases: object

The main Cortix class definition: 1. Create the object 2. Add modules 3. Run the simulation

__del__ ()

Note: 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.

add_module (m)

Add a module to the Cortix object

m: An instance of a class that inherits from the Module base class

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

Draws the networkx Module network graph using matplotlib

file_name: The resulting network diagram output file name *dpi*: dpi used for generating the network image

get_network ()

Constructs and returns a networkx graph representation of the module network.

run ()

Run the Cortix simulation with MPI if available o.w. fallback to multiprocessing

1.2 module module

class module.Module

Bases: object

The representation of a Cortix module. This class is to be inherited by every Cortix module. It provides facilities for creating modules within the Cortix network.

connect (port_name, connected_port)

A simpler interface to create module connectivity. Connect the module port with *port_name* to a given *connected_port*.

get_port (name)

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

recv (port)

Receive data from a given port

run ()

send (*data*, *port*)

Send data through a given port.

1.3 port module

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

Bases: `object`

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.

__eq__ (*other*)

Ports are the same if their names are the same

__repr__ ()

Port name representation

connect (*port*)

Connect the port to another port

port: A Port object that represents the port to connect to.

recv ()

Returns the data recieved from the connected port. NOTE: This function will block until data is received from the connected port

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

Send data to the connected port

data: Any pickelable form of data

EXAMPLES

2.1 dataplot module

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

    plot_data (data_input=None)

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

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

2.2 droplet module

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

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

Note: *external-flow*: this is a *port* that exchanges data with any other module that provides information about the flow outside the droplet.

visualization: this is a *port* that sends data to a visualization module.

```
rhs_fn (u_vec, t, params)
```

```
run ()
```

```
step (time=0.0)
```

ODE IVP problem: Given the initial data at $t = 0$, $(u_1(0), u_2(0), u_3(0)) = (x_0, x_1, x_2)$, $(u_4(0), u_5(0), u_6(0)) = (v_0, v_1, v_2) = (\dot{u}_1(0), \dot{u}_2(0), \dot{u}_3(0))$, solve $\frac{du}{dt} = f(u)$ in the interval $0 \leq t \leq t_f$. When $u_3(t)$ is negative, bounce the droplet to a random height between 0 and 1.0 x_0 with no velocity, and continue the time integration until $t = t_f$.

Parameters **time** (*float*) – Time in the droplet unit of time (seconds).

Returns

Return type None

2.3 dummy_module module

```
class dummy_module.DummyModule
    Bases: cortix.src.module.Module

    run()

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

    run()
```

2.4 plot_data module

```
class plot_data.PlotData
    Bases: cortix.src.module.Module

    run()
```

2.5 run_droplet module

2.6 vortex module

```
class vortex.Vortex
    Bases: cortix.src.module.Module

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

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

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()
```

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.

Parameters `empty` –

Returns `atoms`

Return type `list(str)`

formula

Returns the formula of the chemical in question.

Parameters `empty` –

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__()`

`__str__()`

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.

Parameters **empty** –

Returns **cladding_end_thickness**

Return type **cm**

cladding_mass

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

Parameters **empty** –

Returns **cladding_mass**

Return type **float**

cladding_phase

Returns the phase history of the cladding.

Parameters **empty** –

Returns **cladding_phase**

Return type **dataFrame**

cladding_volume

Returns the total volume of cladding in the bucket, in cm³.

Parameters **empty** –

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.

Parameters **empty** –

Returns **cladding_wall_thickness**

Return type **float**

fresh_u235_mass

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

Parameters **empty** –

Returns **fresh_u235_mass**

Return type **float**

fresh_u238_mass

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

Parameters **empty** –

Returns **fresh_u238_mass**

Return type **float**

fresh_u_mass

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

Parameters **empty** –

Returns **fresh_u_mass**

Return type **float**

fuel_enrichment

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

Parameters **empty** –

Returns **fuel_enrichment**

Return type **float**

fuel_mass

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

Parameters **empty** –

Returns **fuel_mass**

Return type **float**

fuel_mass_unit

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

Parameters **empty** –

Returns **fuel_mass_unit**

Return type **str**

fuel_phase

Returns the phase history of the fuel.

Parameters **empty** –

Returns **fuel_phase**

Return type **pandas.core.frame.DataFrame**

fuel_radioactivity

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

Parameters **empty** –

Returns **fuel_radioactivity**

Return type **float**

fuel_volume

Returns the total volume of fuel in the entire bucket, in cm³.

Parameters **empty** –

Returns **fuel_volume**

Return type **float**

gamma_pwr

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

Parameters **empty** –

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.

Parameters `empty` –

Returns `cladding_end_thickness`

Return type `cm`

get_cladding_mass()

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

Parameters `empty` –

Returns `cladding_mass`

Return type `float`

get_cladding_phase()

Returns the phase history of the cladding.

Parameters `empty` –

Returns `cladding_phase`

Return type `dataFrame`

get_cladding_volume()

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

Parameters `empty` –

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.

Parameters `empty` –

Returns `cladding_wall_thickness`

Return type `float`

get_fresh_u235_mass()

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

Parameters `empty` –

Returns `fresh_u235_mass`

Return type `float`

get_fresh_u238_mass()

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

Parameters `empty` –

Returns `fresh_u238_mass`

Return type `float`

get_fresh_u_mass()

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

Parameters **empty** –

Returns **fresh_u_mass**

Return type **float**

get_fuel_enrichment()

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

Parameters **empty** –

Returns **fuel_enrichment**

Return type **float**

get_fuel_mass()

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

Parameters **empty** –

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.

Parameters **empty** –

Returns **fuel_mass_unit**

Return type **str**

get_fuel_phase()

Returns the phase history of the fuel.

Parameters **empty** –

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.

Parameters **empty** –

Returns **fuel_radioactivity**

Return type **float**

get_fuel_volume()

Returns the total volume of fuel in the entire bucket, in cm³.

Parameters **empty** –

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.

Parameters **empty** –

Returns **gamma_pwr**

Return type **float**

get_heat_pwr()

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

Parameters **empty** –

Returns **heat_pwr**

Return type **float**

get_inner_slug_id()

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

Parameters **empty** –

Returns **inner_slug_id**

Return type **float**

get_inner_slug_od()

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

Parameters **empty** –

Returns **inner_slug_od**

Return type **float**

get_n_slugs()

Returns the number of fuel slugs in the bucket.

Parameters **empty** –

Returns **n_slugs**

Return type **int**

get_name()

Returns the name of the fuel bucket.

Parameters **empty** –

Returns **name**

Return type **str**

get_outer_slug_id()

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

Parameters **empty** –

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.

Parameters **empty** –

Returns **outer_slug_od**

Return type **float**

get_radioactivity()

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

Parameters **empty** –

Returns **radioactivity**

Return type **float**

get_slug_cladding_volume()

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

Parameters **empty** –

Returns **slug_cladding_volume**

Return type **float**

get_slug_fuel_volume()

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

Parameters **empty** –

Returns **slug_fuel_volume**

Return type **float**

get_slug_length()

Returns the length of each slug in the fuel bucket.

Parameters **empty** –

Returns **slug_length**

Return type **float**

get_slug_type()

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

Parameters **empty** –

Returns **slug_type**

Return type **str**

heat_pwr

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

Parameters **empty** –

Returns **heat_pwr**

Return type **float**

inner_slug_id

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

Parameters **empty** –

Returns **inner_slug_id**

Return type **float**

inner_slug_od

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

Parameters **empty** –

Returns **inner_slug_od**

Return type **float**

n_slugs

Returns the number of fuel slugs in the bucket.

Parameters `empty` –

Returns `n_slugs`

Return type `int`

name

Returns the name of the fuel bucket.

Parameters `empty` –

Returns `name`

Return type `str`

outer_slug_id

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

Parameters `empty` –

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.

Parameters `empty` –

Returns `outer_slug_od`

Return type `float`

radioactivity

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

Parameters `empty` –

Returns `radioactivity`

Return type `float`

set_cladding_phase (*phase*)

Set's the phase history to specific values.

Parameters `phase` (*dataFrame*) –

Returns

Return type `empty`

set_fuel_phase (*phase*)

Sets the current fuel phase to a specified phase value.

Parameters `phase` (*dataFrame*) –

Returns

Return type `empty`

set_slug_length (*x*)

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

Parameters `x` (*float*) –

Returns

Return type `empty`

slug_cladding_volume

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

Parameters `empty` –

Returns `slug_cladding_volume`

Return type `float`

slug_fuel_volume

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

Parameters `empty` –

Returns `slug_fuel_volume`

Return type `float`

slug_length

Returns the length of each slug in the fuel bucket.

Parameters `empty` –

Returns `slug_length`

Return type `float`

slug_type

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

Parameters `empty` –

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.

Parameters `empty` –

Returns `fresh_u235_mass`

Return type `float`

fresh_u238_mass

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

Parameters `empty` –

Returns `fresh_u238_mass`

Return type `float`

fresh_u_mass

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

Parameters `empty` –

Returns `fresh_u_mass`

Return type `float`

fuel_enrichment

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

Parameters `empty` –

Returns `fuel_enrichment`

Return type `float`

fuel_mass

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

Parameters `empty` –

Returns `fuel_mass`

Return type `float`

fuel_mass_unit

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

Parameters `empty` –

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.

Parameters `empty` –

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.

Parameters `empty` –

Returns `fuel_pin_volume`

Return type `float`

`fuel_radioactivity`

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

Parameters `empty` –

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.

Parameters `empty` –

Returns `fuel_rod_od`

Return type `float`

`fuel_volume`

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

Parameters `empty` –

Returns `fuel_volume`

Return type `float`

`gamma_pwr`

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

Parameters `empty` –

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.

Parameters `empty` –

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.

Parameters `empty` –

Returns `gas_radioactivity`

Return type `float`

`get_fresh_U235_mass()`

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

Parameters `empty` –

Returns `fresh_u235_mass`

Return type `float`

get_fresh_u238_mass()

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

Parameters **empty** –

Returns **fresh_u238_mass**

Return type **float**

get_fresh_u_mass()

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

Parameters **empty** –

Returns **fresh_u_mass**

Return type **float**

get_fuel_enrichment()

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

Parameters **empty** –

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.

Parameters **empty** –

Returns **fuel_mass**

Return type **float**

get_fuel_mass_unit()

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

Parameters **empty** –

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.

Parameters **empty** –

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.

Parameters **empty** –

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.

Parameters `empty` –

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.

Parameters `empty` –

Returns `fuel_rod_od`

Return type `float`

get_fuel_volume()

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

Parameters `empty` –

Returns `fuel_volume`

Return type `float`

get_gamma_pwr()

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

Parameters `empty` –

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.

Parameters `empty` –

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.

Parameters `empty` –

Returns `gas_radioactivity`

Return type `float`

get_heat_pwr()

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

Parameters `empty` –

Returns `heat_pwr`

Return type `float`

get_n_fuel_rods()

Returns the number of fuel rods in the bundle.

Parameters `empty` –

Returns `n_fuel_rods`

Return type `int`

get_name()

Returns the name of the fuel bundle.

Parameters `empty` –

Returns `name`

Return type `str`

get_radioactivity()

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

Parameters `empty` –

Returns `radioactivity`

Return type `float`

get_solid_phase()

Returns the solid phase history associated with this fuel bundle.

Parameters `empty` –

Returns `solidPhase`

Return type `dataFrame`

heat_pwr

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

Parameters `empty` –

Returns `heat_pwr`

Return type `float`

n_fuel_rods

Returns the number of fuel rods in the bundle.

Parameters `empty` –

Returns `n_fuel_rods`

Return type `int`

name

Returns the name of the fuel bundle.

Parameters `empty` –

Returns `name`

Return type `str`

radioactivity

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

Parameters `empty` –

Returns `radioactivity`

Return type `float`

set_fuel_pin_length (*x*)

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

Parameters **empty** –

Returns *x*

Return type *float*

set_gas_phase (*phase*)

Sets the gas phase history of the fuel equal to *phase*.

Parameters **phase** (*dataFrame*) –

Returns

Return type *empty*

set_solid_phase (*phase*)

Sets the solid phase history of the fuel equal to *phase*.

Parameters **phase** (*dataFrame*) –

Returns

Return type *empty*

solid_phase

Returns the solid phase history associated with this fuel bundle.

Parameters **empty** –

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.

Parameters **empty** –

Returns *s*

Return type *str*

__str__ ()

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

Parameters **empty** –

Returns *s*

Return type *str*

geometry

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

Parameters **Empty** –

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).

Parameters **Empty** –

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. :param None:

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. :param None:

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*) –

Returns

Return type empty

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.

Parameters empty –

Returns claddingPhase

Return type dataframe

GetFuelPhase ()

Returns the phase history of the solid fuel.

Parameters empty –

Returns fuelPhase

Return type dataframe

GetSpecs ()

Returns the species associated with this fuel slug.

Parameters empty –

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*) –

Returns

Return type empty

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*) –

Returns

Return type empty

claddingPhase

Returns the phase history of the cladding.

Parameters empty –

Returns claddingPhase

Return type dataframe

fuelPhase

Returns the phase history of the solid fuel.

Parameters `empty` –

Returns `fuelPhase`

Return type `dataFrame`

specs

Returns the species associated with this fuel slug.

Parameters `empty` –

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*) –

Returns**Return type** empty**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*) –

Returns**Return type** empty**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*) –**Returns****Return type** empty**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*) –**Returns****Return type** empty**GetActors** ()

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

Parameters **empty** –**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[``actor])`: `list`**GetQuantities** ()

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

Parameters **empty** –**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*) –

Returns**Return type** empty**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.

Parameters *empty* –**Returns** *species***Return type** *list***GetTimeStamps** ()

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

Parameters *empty* –**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*) –**Returns****Return type** empty**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*) –**Returns**

Return type empty

SetSpecieId (*name*, *val*)

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

Parameters

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

Returns

Return type empty

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*) –

Returns

Return type empty

WriteHTML (*fileName*)

Convert the *Phase* container into an HTML file.

Parameters **fileName** (*str*) –

Returns

Return type empty

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*,*float*)

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.

Parameters **empty** –

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.

Parameters **empty** –

Returns **species**

Return type *list*

timeStamps

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

Parameters **empty** –

Returns **timeStamps**

Return type *list*

time_stamps

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

Parameters **empty** –

Returns **time_stamps**

Return type *list*

time_unit

Returns the time unit of the *Phase*.

Parameters **empty** –

Returns **time_unit**

Return type *str*

3.10 quantity

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

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.

GetFormalName()

Returns the formal name of the quantity.

Parameters `empty` –

Returns `formalName`

Return type `str`

GetUnit()

Returns the units of the quantity.

Parameters `empty` –

Returns `unit`

Return type `str`

GetValue()

Gets the numerical value of the quantity.

Parameters `empty` –

Returns `value`

Return type `float`

SetFormalName(fn)

Sets the formal name of the property to fn.

Parameters `fn(str)` –

Returns

Return type `empty`

SetName(n)

Sets the name of the quantity in question to n.

Parameters `n(str)` –

Returns

Return type `empty`

SetUnit(f)

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

Parameters `f(str)` –

Returns

Return type empty

SetValue (*v*)

Sets the numerical value of the quantity to *v*.

Parameters *v* (*float*) –

Returns

Return type empty

__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.

Parameters empty –

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.

Parameters empty –

Returns *s*

Return type *str*

formalName

Returns the formal name of the quantity.

Parameters empty –

Returns *formalName*

Return type *str*

formal_name

Returns the formal name of the quantity.

Parameters empty –

Returns *formalName*

Return type *str*

get_name ()

Returns the name of the quantity.

Parameters empty –

Returns *name*

Return type *str*

name

Returns the name of the quantity.

Parameters empty –

Returns *name*

Return type *str*

unit

Returns the units of the quantity.

Parameters `empty` –

Returns `unit`

Return type `str`

value

Gets the numerical value of the quantity.

Parameters `empty` –

Returns `value`

Return type `float`

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 hipphen 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.

Parameters `empty` –

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".

Parameters `empty` –

Returns `self.__formula_name`

Return type `str`

GetMassCC()

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

Parameters `empty` –

Returns `massCC`

Return type `float`

GetMassCCUnit()

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

Parameters `empty` –

Returns `massCCUnit`

Return type `str`

GetMolarCC()

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

Parameters `empty` –

Returns `molarCC`

Return type `float`

GetMolarCCUnit()

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

Parameters `empty` –

Returns `molarCCUnit`

Return type `str`

GetMolarGammaPwr()

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

Parameters `empty` –

Returns `molarGammaPwr`

Return type `float`

GetMolarGammaPwrUnit ()

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

Parameters `empty` –

Returns `molarGammaPwrUnit`

Return type `str`

GetMolarHeatPwr ()

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

Parameters `empty` –

Returns `molarHeatPwr`

Return type `float`

GetMolarHeatPwrUnit ()

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

Parameters `empty` –

Returns `molarHeatPwrUnit`

Return type `str`

GetMolarMass ()

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

Parameters `empty` –

Returns `molarMass`

Return type `float`

GetMolarMassUnit ()

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

Parameters `empty` –

Returns `molarMassUnit`

Return type `str`

GetMolarRadioactivity ()

Returns the numerical value for molar radioactivity of the species.

Parameters `empty` –

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.

Parameters `empty` –

Returns `molarRadioactivityFractions`

Return type `list`

GetMolarRadioactivityUnit ()

Returns the unit used to measure molar radioactivity.

Parameters `empty` –

Returns `molarRadioactivityUnit`

Return type `str`

GetNAtoms ()

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

Parameters `empty` –

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.

Parameters `empty` –

Returns `nNuclideTypes`

Return type `int`

GetName ()

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

Parameters `empty` –

Returns `name`

Return type `str`

GetPhase ()

Returns the phase history of the species.

Parameters `empty` –

Returns `phase`

Return type `dataFrame`

SetAtoms (*atoms*)**SetFlag (*f*)**

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

Parameters *f* (`str`) –

Returns

Return type `empty`

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`) –

Returns

Return type `empty`

SetFormulaName (*f*)

Sets the formulaic name to *f*.

Parameters *empty* –

Returns

- *empty*
- **self.__formula_name** (*str*)

SetMassCC (*v*)

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

Parameters *v* (*float*) –

Returns

Return type *empty*

SetMassCCUnit (*v*)

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

Parameters *v* (*str*) –

Returns

Return type *empty*

SetMolarCC (*v*)

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

Parameters *v* (*float*) –

Returns

Return type *empty*

SetMolarCCUnit (*v*)

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

Parameters *v* (*str*) –

Returns

Return type *empty*

SetMolarGammaPwr (*v*)

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

Parameters *v* (*float*) –

Returns

Return type *empty*

SetMolarGammaPwrUnit (*v*)

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

Parameters *v* (*str*) –

Returns

Return type *empty*

SetMolarHeatPwr (*v*)

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

Parameters *v* (*float*) –

Returns**Return type** empty**SetMolarHeatPwrUnit** (*v*)Sets the unit used to measure the amount of heat generated per mole of this species to *v*.**Parameters** *v* (*str*) –**Returns****Return type** empty**SetMolarMass** (*v*)Sets the molar mass of the species equal to *v*.**Parameters** *v* (*float*) –**Returns****Return type** empty**SetMolarMassUnit** (*v*)Sets the unit used to measure the molar mass of the species to *v*.**Parameters** *v* (*str*) –**Returns****Return type** empty**SetMolarRadioactivity** (*v*)Sets the molar radioactivity of the species equal to *v*.**Parameters** *v* (*float*) –**Returns****Return type** empty**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*) –**Returns****Return type** empty**SetMolarRadioactivityUnit** (*v*)Sets the unit used to measure molar radioactivity to *v*.**Parameters** *v* (*str*) –**Returns****Return type** empty**SetName** (*n*)Sets the empirical name of the species to *n*.**Parameters** *n* (*str*) –**Returns**

Return type `empty`

SetPhase (*p*)

Sets the phase history to *p*.

Parameters *p* (*dataFrame*) –

Returns

Return type `empty`

atoms

flag

Returns the flag associated with the species.

Parameters `empty` –

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".

Parameters `empty` –

Returns `self.__formula_name`

Return type `str`

massCC

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

Parameters `empty` –

Returns `massCC`

Return type `float`

massCCUnit

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

Parameters `empty` –

Returns `massCCUnit`

Return type `str`

molarCC

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

Parameters `empty` –

Returns `molarCC`

Return type `float`

molarCCUnit

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

Parameters **empty** –

Returns **molarCCUnit**

Return type **str**

molarGammaPwr

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

Parameters **empty** –

Returns **molarGammaPwr**

Return type **float**

molarGammaPwrUnit

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

Parameters **empty** –

Returns **molarGammaPwrUnit**

Return type **str**

molarHeatPwr

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

Parameters **empty** –

Returns **molarHeatPwr**

Return type **float**

molarHeatPwrUnit

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

Parameters **empty** –

Returns **molarHeatPwrUnit**

Return type **str**

molarMass

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

Parameters **empty** –

Returns **molarMass**

Return type **float**

molarMassUnit

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

Parameters **empty** –

Returns **molarMassUnit**

Return type **str**

molarRadioactivity

Returns the numerical value for molar radioactivity of the species.

Parameters **empty** –

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.

Parameters `empty` –

Returns `molarRadioactivityFractions`

Return type `list`

molarRadioactivityUnit

Returns the unit used to measure molar radioactivity.

Parameters `empty` –

Returns `molarRadioactivityUnit`

Return type `str`

nAtoms

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

Parameters `empty` –

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.

Parameters `empty` –

Returns `nNuclideTypes`

Return type `int`

name

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

Parameters `empty` –

Returns `name`

Return type `str`

phase

Returns the phase history of the species.

Parameters `empty` –

Returns `phase`

Return type `dataFrame`

3.12 stream

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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.

Parameters **empty** –

Returns `list(self.stream.columns)`

Return type `list`

GetQuantities ()

Returns all the quantities given by the stream.

Parameters **empty** –

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.

Parameters **empty** –

Returns `self.species`

Return type `list`

GetTimeStamp ()

Returns the time stamp of the stream.

Parameters **empty** –

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*) –

Returns

Return type `empty`

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*) –

Returns

Return type `empty`

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