
numericalmodel Documentation

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What is `numericalmodel`?

The Python package `numericalmodel` is an attempt to **make prototyping simple numerical models** in Python an **easy and painless** task.

Why should I prototype a numerical model in Python?

During development phase of a model, it is very handy to be able to flexibly change crucial model parts. One might want to quickly:

- add more **variables/parameters/forcings**
- add another **model equation**
- have specific **forcings be time-dependent**
- test another **numerical scheme**
- use **different numerical schemes for each equation**
- **combine numerical schemes** to solve different equation parts
- etc.

Quickly achieving this in a compiled, inflexible language like **Fortran** or **C** may not be that easy. Also, debugging or unit testing such a language is way more inconvenient than it is in Python. With Python, one can take advantage of the extreme flexibility that object orientation and object introspection provides.

While it is obvious, that such a prototyped model written in an interpreted language like Python will never come up to the speed and efficiency of a compiled language, it may seem very appealing in terms of flexibility. Once it's clear how the model should look like and fundamental changes are unlikely to occur anymore, it can be translated into another, faster language.

Can I implement any numerical model with `numericalmodel`?

No, at least for now :-). Currently, there are a couple of restrictions:

- **only zero-dimensional models** are supported for now. Support for more dimensions is on the TODO-list.
- `numericalmodel` is focused on **physical models**

But that doesn't mean that you can't create new subclasses from `numericalmodel` to fit your needs.

Is setting up a numerical model with `numericalmodel` really that easy?

Have a look at the *Basics*, *Setting up a model* and the *Examples* and see for yourself.

CHAPTER 2

Installation

numericalmodel is best installed via pip:

```
pip3 install --user numericalmodel
```


Basic structure

The basic model structure is assumed the following:

- The model itself (*NumericalModel*) knows:
 - some metadata
 - the variables (*SetOfStateVariables*)
 - the parameters (*SetOfParameters*)
 - the forcing (*SetOfForcingValues*)
 - the numerical schemes (*SetOfNumericalSchemes*)
 - *[output facilities]*
- The numerical schemes (*SetOfNumericalSchemes*) know:
 - the individual numerical schemes (*NumericalScheme*) each for a specific equation (*Equation*)
 - how to integrate their equations (*NumericalScheme.integrate*)
- The equations (*SetOfEquations*) know:
 - the equation variable (*StateVariable*)
 - the equation input (*SetOfInterfaceValues*) - which may contain other variables
 - how to calculate the equation (e.g. the linear and nonlinear part of a derivative)

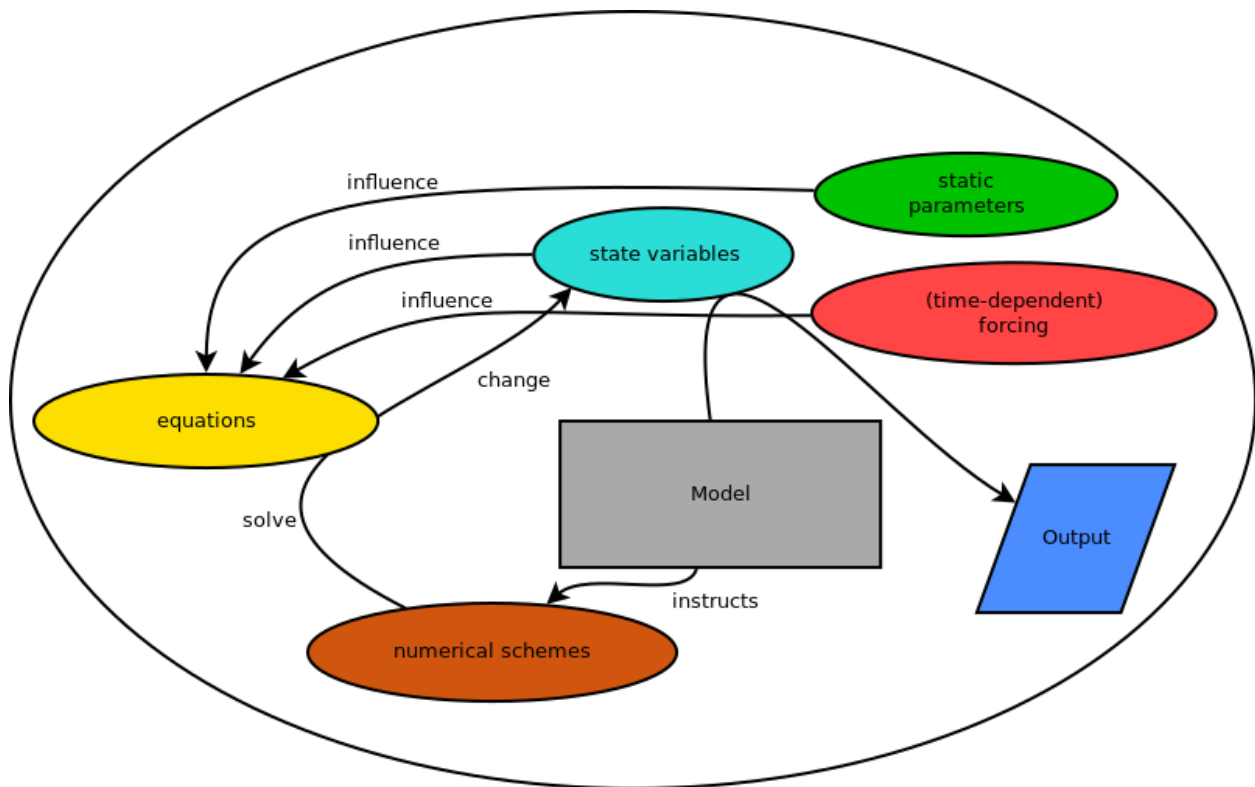


Fig. 3.1: The basic model structure

CHAPTER 4

Setting up a model

We are going to implement a simple linear decay equation:

$$\frac{dT}{dt} = -a \cdot T + F$$

Where T is the temperature in Kelvin, $a > 0$ is the linear constant and F the forcing parameter.

To set up the model, some straight-forward steps are necessary. First, import the *numericalmodel* module:

```
import numericalmodel
```

Creating a model

First initialize an object of *NumericalModel*:

```
model = numericalmodel.numericalmodel.NumericalModel()
```

We may tell the model to start from time 0:

```
model.initial_time = 0
```

Defining variables, parameters and forcing

The *StateVariable*, *Parameter*, and *ForcingValue* classes all derive from *InterfaceValue*, which is a convenient class for time/value management. It also provides interpolation (*InterfaceValue.__call__*). An *InterfaceValue* has a (sensibly unique) *id* for it to be referencable in a *SetOfInterfaceValues*.

For convenience, let's import everything from the *interfaces* submodule:

```
from numericalmodel.interfaces import *
```

Let's define our state variable. For the simple case of the linear decay equation, our only state variable is the temperature T :

```
temperature = StateVariable( id = "T", name = "temperature", unit = "K" )
```

Providing a name and a unit documents your model on the fly.

Tip: All classes in *numericalmodel* are subclasses of *ReprObject*. This makes them have a proper `__repr__` method to provide an as-exact-as-possible representation. So at any time you might do a `print(repr(temperature))` or just `temperature<ENTER>` in an interactive python session to see a representation of this object:

```
numericalmodel.interfaces.StateVariable(  
    time_function = numericalmodel.utils.utcnw,  
    values = array([], dtype=float64),  
    name = 'temperature',  
    times = array([], dtype=float64),  
    unit = 'K',  
    id = 'T',  
    interpolation = 'zero'  
)
```

The others - a and F - are created similarly:

```
parameter = Parameter( id = "a", name = "linear parameter", unit = "1/s" )  
forcing = ForcingValue( id = "F", name = "forcing parameter", unit = "K/s" )
```

Now we add them to the model:

```
model.variables = SetOfStateVariables( [ temperature ] )  
model.parameters = SetOfParameters( [ parameter ] )  
model.forcing = SetOfForcingValues( [ forcing ] )
```

Tip: A lot of objects in *numericalmodel* also have a sensible `__str__` method, which enables them to print a summary of themselves. For example, if we do a `print(model)`:

```
###  
### "numerical model"  
### - a numerical model -  
### version 0.0.1  
###  
  
by:  
anonymous  
  
a numerical model  
-----  
This is a numerical model.  
  
  
#####  
### Model data ###  
#####
```

```
initial time: 1490648927.012074
```

```
#####
### Variables ###
#####
```

```
    "temperature"
--- T [K] ---
currently: ? [K]
interpolation: zero
0 total recorded values
```

```
#####
### Parameters ###
#####
```

```
    "linear parameter"
--- a [1/s] ---
currently: ? [1/s]
interpolation: linear
0 total recorded values
```

```
#####
### Forcing ###
#####
```

```
    "forcing parameter"
--- F [K/s] ---
currently: ? [K/s]
interpolation: linear
0 total recorded values
```

```
#####
### Schemes ###
#####
```

```
none
```

Note: When an *InterfaceValue*'s *value* is set, a corresponding time is determined to record it. The default is to use the return value of the *InterfaceValue.time_function*, which in turn defaults to the current utc timestamp. When the model was told to use temperature, parameter and forcing, it automatically set the *InterfaceValue.time_function* to its internal *model_time*. That's why it makes sense to define initial values **after** adding the *InterfaceValue*s to the model.

Now that we have defined our model and added the variables, parameters and forcing, we may set initial values:

```
temperature.value = 20 + 273.15
parameter.value   = 0.1
forcing.value     = 28
```

Tip: We could also have made use of *SetOfInterfaceValues*' handy indexing features and have said:

```
model.variables["T"].value = 20 + 273.15
model.parameters["a"].value = 0.1
model.forcing["F"].value = 28
```

Defining equations

We proceed by defining our equation. In our case, we do this by subclassing *PrognosticEquation*, since the linear decay equation is a prognostic equation:

```
class LinearDecayEquation(numericalmodel.equations.PrognosticEquation):
    """
    Class for the linear decay equation
    """
    def linear_factor(self, time = None):
        # take the "a" parameter from the input, interpolate it to the given
        # "time" and return the negative value
        return - self.input["a"](time)

    def independent_addend(self, time = None):
        # take the "F" forcing parameter from the input, interpolate it to
        # the given "time" and return it
        return self.input["F"](time)

    def nonlinear_addend(self, *args, **kwargs):
        return 0 # nonlinear addend is always zero (LINEAR decay equation)
```

Now we initialize an object of this class:

```
decay_equation = LinearDecayEquation(
    variable = temperature,
    input = SetOfInterfaceValues( [parameter, forcing] ),
)
```

We can now calculate the derivative of the equation with the *derivative* method:

```
>>> decay_equation.derivative()
-28.314999999999998
```

Choosing numerical schemes

Alright, we have all input we need and an equation. Now everything that's missing is a numerical scheme to solve the equation. *numericalmodel* ships with the most common numerical schemes. They reside in the submodule *numericalmodel.numericalschemes*. For convenience, we import everything from there:

```
from numericalmodel.numericalschemes import *
```

For a linear decay equation whose parameters are independent of time, the *EulerImplicit* scheme is a good choice:

```
implicit_scheme = numericalmodel.numericalschemes.EulerImplicit(
    equation = decay_equation
)
```

We may now add the scheme to the model:

```
model.numericalschemes = SetOfNumericalSchemes( [ implicit_scheme ] )
```

That's it! The model is ready to run!

Running the model

Running the model is as easy as telling it a final time:

```
model.integrate( final_time = model.model_time + 60 )
```

Model results

The model results are written directly into the *StateVariable*'s cache. You may either access the values directly via the *values* property (a *numpy.ndarray*) or interpolated via the *InterfaceValue.__call__* method.

One may plot the results with *matplotlib.pyplot*:

```
import matplotlib.pyplot as plt

plt.plot( temperature.times, temperature.values,
          linewidth = 2,
          label = temperature.name,
          )
plt.xlabel( "time [seconds]" )
plt.ylabel( "{} [{}].format( temperature.name, temperature.unit ) )
plt.legend()
plt.show()
```

The full code can be found in the *Examples* section.

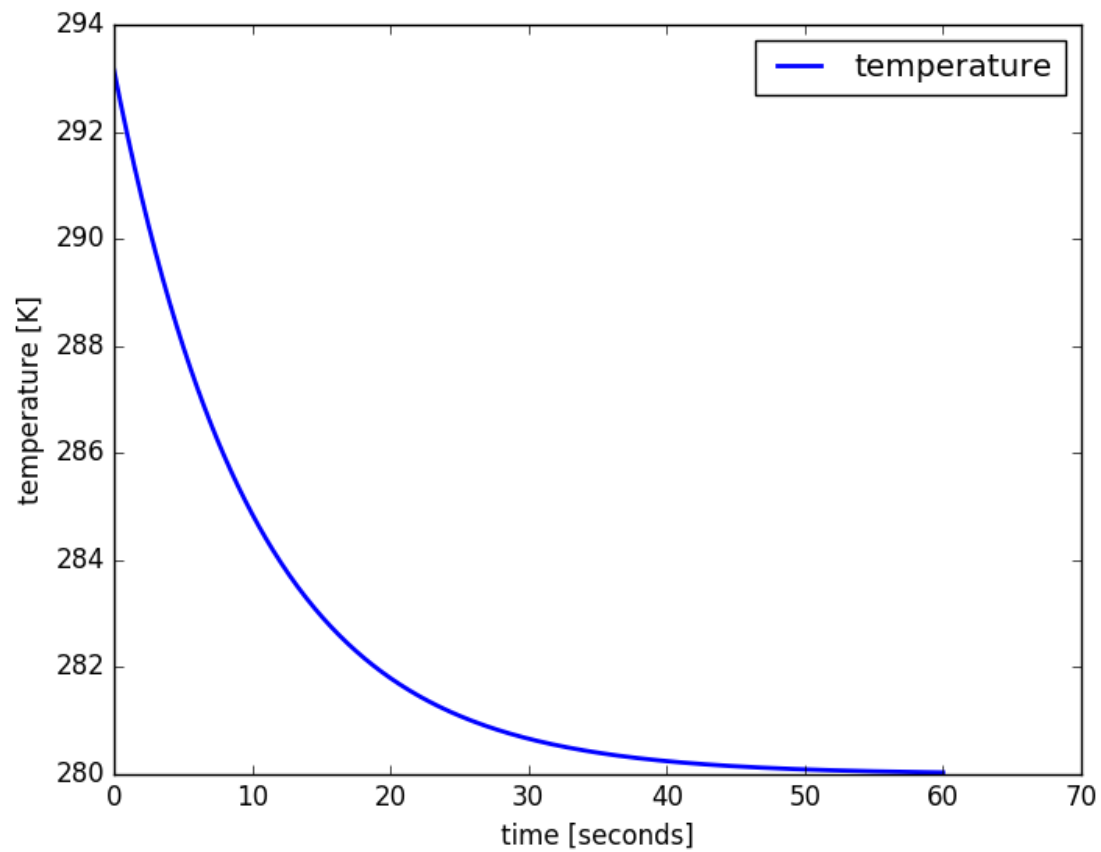


Fig. 4.1: The linear decay model results

Linear decay equation

This is the full code from the *Setting up a model* section:

```
# import the module
import numericalmodel
from numericalmodel.interfaces import *
from numericalmodel.numericalschemes import *

# create a model
model = numericalmodel.numericalmodel.NumericalModel()
model.initial_time = 0

# define values
temperature = StateVariable( id = "T", name = "temperature", unit = "K" )
parameter = Parameter( id = "a", name = "linear parameter", unit = "1/s" )
forcing = ForcingValue( id = "F", name = "forcing parameter", unit = "K/s" )

# add the values to the model
model.variables = SetOfStateVariables( [ temperature ] )
model.parameters = SetOfParameters( [ parameter ] )
model.forcing = SetOfForcingValues( [ forcing ] )

# set initial values
model.variables["T"].value = 20 + 273.15
model.parameters["a"].value = 0.1
model.forcing["F"].value = 28

# define the equation
class LinearDecayEquation(numericalmodel.equations.PrognosticEquation):
    """
    Class for the linear decay equation
    """
    def linear_factor(self, time = None ):
```

```
# take the "a" parameter from the input, interpolate it to the given
# "time" and return the negative value
return - self.input["a"](time)

def independent_addend(self, time = None ):
    # take the "F" forcing parameter from the input, interpolate it to
    # the given "time" and return it
    return self.input["F"](time)

def nonlinear_addend(self, *args, **kwargs):
    return 0 # nonlinear addend is always zero (LINEAR decay equation)

# create an equation object
decay_equation = LinearDecayEquation(
    variable = temperature,
    input = SetOfInterfaceValues( [parameter, forcing] ),
)

# create a numerical scheme
implicit_scheme = numericalmodel.numericalschemes.EulerImplicit(
    equation = decay_equation
)

# add the numerical scheme to the model
model.numericalschemes = SetOfNumericalSchemes( [ implicit_scheme ] )

# integrate the model
model.integrate( final_time = model.model_time + 60 )

# plot the results
import matplotlib.pyplot as plt

plt.plot( temperature.times, temperature.values,
          linewidth = 2,
          label = temperature.name,
          )
plt.xlabel( "time [seconds]" )
plt.ylabel( "{} [{}].format( temperature.name, temperature.unit ) )
plt.legend()
plt.show()
```

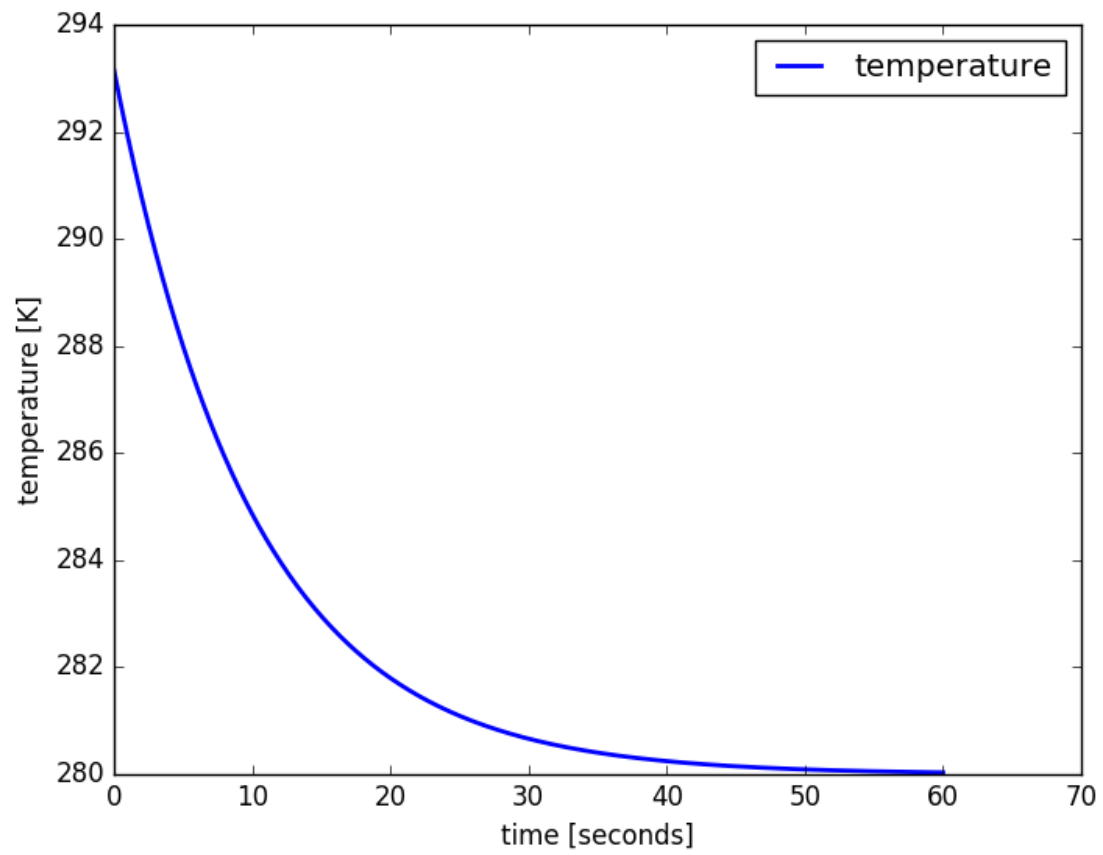


Fig. 5.1: The linear decay model results

numericalmodel package

numericalmodel Python module

Submodules

numericalmodel.equations module

class `numericalmodel.equations.DerivativeEquation` (*variable=None, description=None, long_description=None, input=None*)

Bases: `numericalmodel.equations.Equation`

Class to represent a derivative equation

derivative (*time=None, variablevalue=None*)

Calculate the derivative (right-hand-side) of the equation

Parameters

- **times** (*single numeric value, optional*) – the time to calculate the derivative. Defaults to the variable’s current (last) time.
- **variablevalue** (*np.array, optional*) – the variable value to use. Defaults to the value of `self.variable` at the given time.

Returns the derivatives corresponding to the given time

Return type `numpy.ndarray`

independent_addend (*time=None*)

Calculate the derivative’s addend part that is independent of the variable.

Parameters **times** (*single numeric value, optional*) – the time to calculate the derivative. Defaults to the variable’s current (last) time.

Returns the equation's variable-independent addend at the corresponding time

Return type `numpy.array`

linear_factor (*time=None*)

Calculate the derivative's linear factor in front of the variable

Parameters **time** (*single numeric value, optional*) – the time to calculate the derivative. Defaults to the variable's current (last) time.

Returns the equation's linear factor at the corresponding time

Return type `numpy.array`

nonlinear_addend (*time=None, variablevalue=None*)

Calculate the derivative's addend part that is nonlinearly dependent of the variable.

Parameters

- **times** (*single numeric value, optional*) – the time to calculate the derivative. Defaults to the variable's current (last) time.
- **variablevalue** (*np.array, optional*) – the variable value to use. Defaults to the value of `self.variable` at the given time.

Returns the equation's nonlinear addend at the corresponding time

Return type `numpy.array`

class `numericalmodel.equations.DiagnosticEquation` (*variable=None, description=None, long_description=None, input=None*)

Bases: `numericalmodel.equations.Equation`

Class to represent diagnostic equations

class `numericalmodel.equations.Equation` (*variable=None, description=None, long_description=None, input=None*)

Bases: `numericalmodel.utils.LoggerObject`, `numericalmodel.utils.ReprObject`

Base class for equations

Parameters

- **description** (*str, optional*) – short equation description
- **long_description** (*str, optional*) – long equation description
- **variable** (*StateVariable, optional*) – the variable obtained by solving the equation
- **input** (*SetOfInterfaceValues, optional*) – set of values needed by the equation

__str__ ()

Stringification

Returns a summary

Return type `str`

depends_on (*id*)

Check if this equation depends on a given `InterfaceValue`

Parameters **id** (*str or InterfaceValue*) – an `InterfaceValue` or an `id`

Returns True if 'id' is in `input`, False otherwise

Return type `bool`

description

The description of the equation

Type `str`

input

The input needed by the equation. Only real dependencies should be included. If the equation depends on the *variable*, it should also be included in *input*.

Type `SetOfInterfaceValues`

long_description

The longer description of this equation

Type `str`

variable

The variable the equation is able to solve for

Type `StateVariable`

class `numericalmodel.equations.PrognosticEquation` (*variable=None, description=None, long_description=None, input=None*)

Bases: `numericalmodel.equations.DerivativeEquation`

Class to represent prognostic equations

class `numericalmodel.equations.SetOfEquations` (*elements=[]*)

Bases: `numericalmodel.utils.SetOfObjects`

Base class for sets of Equations

Parameters *elements* (*list of Equations, optional*) – the list of *Equation* instances

_object_to_key (*obj*)

key transformation function.

Parameters *obj* (*object*) – the element

Returns the unique key for this object. The *Equation.variable*'s *id* is used.

Return type `str`

numericalmodel.genericmodel module

class `numericalmodel.genericmodel.GenericModel` (*name=None, version=None, description=None, long_description=None, authors=None*)

Bases: `numericalmodel.utils.LoggerObject, numericalmodel.utils.ReprObject`

Base class for models

Parameters

- **name** (*str, optional*) – the model name
- **version** (*str, optional*) – the model version
- **description** (*str*) – a short model description
- **long_description** (*str*) – an extended model description
- **authors** (*str, list or dict, optional*) – model authors. *str*: name of single author *list*: list of author names *dict*: dict of {'task': ['name1', 'name1']} pairs

`__str__()`

Stringification

Returns a summary

Return type `str`

authors

The model author(s)

One of:

- `str` : one author
- `list` of `str` : multiple authors
- `Dictionary displays` : multiple authors per task, e.g. { "task1" : ["author1", "author2"], "task2" : ... }

description

The model description

Type `str`

long_description

Longer model description

Type `str`

name

The model name

Type `str`

version

The model version

Type `str`

numericalmodel.interfaces module

```
class numericalmodel.interfaces.ForcingValue (name=None, id=None, unit=None,
                                              time_function=None, interpolation=None,
                                              values=None, times=None)
```

Bases: `numericalmodel.interfaces.InterfaceValue`

Class for forcing values

```
class numericalmodel.interfaces.InterfaceValue (name=None, id=None, unit=None,
                                              time_function=None, interpolation=None,
                                              values=None, times=None)
```

Bases: `numericalmodel.utils.LoggerObject`, `numericalmodel.utils.ReprObject`

Base class for model interface values

Parameters

- **name** (`str`) – value name
- **id** (`str`) – unique id
- **values** (`1d np.array`) – all values this InterfaceValue had in chronological order
- **times** (`1d np.array`) – the corresponding times to values
- **unit** (`str`) – physical unit of value

- **interpolation** (*str*) – interpolation kind. See `scipy.interpolate.interp1d` for documentation. Defaults to “zero”.
- **time_function** (*callable*) – function that returns the model time as utc unix timestamp

__call__ (*times=None*)

When called, return the value, optionally at a specific time

Parameters **times** (*numeric, optional*) – The times to obtain data from

__str__ ()

Stringification

Returns a summary

Return type *str*

id

The unique id

Type *str*

interpolation

The interpolation kind to use in the **__call__** method. See `scipy.interpolate.interp1d` for documentation.

Getter Return the interpolation kind.

Setter Set the interpolation kind. Reset the internal interpolator if the interpolation kind changed.

Type *str*

interpolator

The interpolator for interpolation of *values* over *times*. Creating this interpolator is costly and thus only performed on demand, i.e. when **__call__** is called **and** no interpolator was created previously or the previously created interpolator was unset before (e.g. by setting a new *value* or changing *interpolation*)

Type `scipy.interpolate.interp1d`

name

The name.

Type *str*

next_time

The next time to use when *value* is set.

Getter Return the next time to use. Defaults to the value of *time_function* if no *next_time* was set.

Setter Set the next time to use. Set to `None` to unset and use the default time in the getter again.

Type *float*

time

The current time

Getter Return the current time, i.e. the last time recorded in *times*.

Type *float*

time_function

times

All times the *value* has ever been set in chronological order

Type `numpy.ndarray`

unit

The SI-unit.

Type `str`, SI-unit

value

The current value.

Getter the return value of `__call__`, i.e. the current value.

Setter When this property is set, the given value is recorded to the time given by *next_time*. If this time exists already in *times*, the corresponding value in *values* is overwritten. Otherwise, the new time and value are appended to *times* and *values*.

Type numeric

values

All values this InterfaceValue has ever had in chronological order

Type `numpy.ndarray`

class `numericalmodel.interfaces.Parameter` (*name=None, id=None, unit=None, time_function=None, interpolation=None, values=None, times=None*)

Bases: `numericalmodel.interfaces.InterfaceValue`

Class for parameters

class `numericalmodel.interfaces.SetOfForcingValues` (*elements=[]*)

Bases: `numericalmodel.interfaces.SetOfInterfaceValues`

Class for a set of forcing values

class `numericalmodel.interfaces.SetOfInterfaceValues` (*elements=[]*)

Bases: `numericalmodel.utils.SetOfObjects`

Base class for sets of interface values

Parameters *values* (*list of value_type-instances, optional*) – the list of values

__call__ (*id*)

Get the value of an *InterfaceValue* in this set

Parameters *id* (*str*) – the id of an *InterfaceValue* in this set

Returns the *value* of the corresponding *InterfaceValue*

Return type `float`

_object_to_key (*obj*)

key transformation function.

Parameters *obj* (*object*) – the element

Returns the unique key for this object. The *InterfaceValue.id* is used.

Return type `key (str)`

time_function

The time function of all the *InterfaceValue*s in the set.

Getter Return a *list* of time functions from the elements

Setter Set the time function of each element

Type (list of) callables

class `numericalmodel.interfaces.SetOfParameters` (*elements=[]*)

Bases: `numericalmodel.interfaces.SetOfInterfaceValues`

Class for a set of parameters

class `numericalmodel.interfaces.SetOfStateVariables` (*elements=[]*)

Bases: `numericalmodel.interfaces.SetOfInterfaceValues`

Class for a set of state variables

class `numericalmodel.interfaces.StateVariable` (*name=None, id=None, unit=None, time_function=None, interpolation=None, values=None, times=None*)

Bases: `numericalmodel.interfaces.InterfaceValue`

Class for state variables

numericalmodel.numericalmodel module

class `numericalmodel.numericalmodel.NumericalModel` (*name=None, version=None, description=None, long_description=None, authors=None, initial_time=None, parameters=None, forcing=None, variables=None, numericalschemes=None*)

Bases: `numericalmodel.genericmodel.GenericModel`

Class for numerical models

Parameters

- **name** (*str, optional*) – the model name
- **version** (*str, optional*) – the model version
- **description** (*str, optional*) – a short model description
- **long_description** (*str, optional*) – an extended model description
- **authors** (*str, list or dict, optional*) – model authors. str: name of single author list: list of author names dict: dict of {'task': ['name1', 'name1']} pairs
- **initial_time** (*float*) – initial model time (UTC unix timestamp)
- **parameters** (*SetOfParameters, optional*) – model parameters
- **forcing** (*SetOfForcingValues, optional*) – model forcing
- **variables** (*SetOfStateVariables, optional*) – model state variables
- **numericalschemes** (*SetOfNumericalSchemes, optional*) – model schemes with equation

__str__ ()

Stringification

Returns a summary

Return type *str*

forcing
The model forcing
Type *SetOfForcingValues*

get_model_time()
The current model time
Returns current model time
Return type *float*

initial_time
The initial model time
Type *float*

integrate(*final_time*)
Integrate the model until *final_time*
Parameters **final_time** (*float*) – time to integrate until

model_time
The current model time
Type *float*

numericalschemes
The model numerical schemes
Type *str*

parameters
The model parameters
Type *SetOfParameters*

variables
The model variables
Type *SetOfStateVariables*

numericalmodel.numericalschemes module

```
class numericalmodel.numericalschemes.EulerExplicit (description=None,
long_description=None,
equation=None,
back_max_timestep=None,
ignore_linear=None,
ignore_independent=None,
ignore_nonlinear=None)

Bases: numericalmodel.numericalschemes.NumericalScheme

Euler-explicit numerical scheme

step (time=None, timestep=None, tendency=True)
```

```
class numericalmodel.numericalschemes.EulerImplicit (description=None,
                                                    long_description=None,
                                                    equation=None,          fall-
                                                    back_max_timestep=None,
                                                    ignore_linear=None,         ig-
                                                    nore_independent=None,         ig-
                                                    nore_nonlinear=None)
```

Bases: `numericalmodel.numericalschemes.NumericalScheme`

Euler-implicit numerical scheme

step (*time=None, timestep=None, tendency=True*)

Integrate one “timestep” from “time” forward with the Euler-implicit scheme and return the resulting variable value.

Parameters

- **time** (*single numeric*) – The time to calculate the step FROM
- **timestep** (*single numeric*) – The timestep to calculate the step
- **tendency** (*bool, optional*) – return the tendency or the actual value of the variable after the timestep?

Returns The resulting variable value or tendency

Return type `numpy.ndarray`

Raises `AssertionError` – when the equation’s nonlinear part is not zero and `ignore_nonlinear` is not set to True

```
class numericalmodel.numericalschemes.LeapFrog (description=None, long_description=None,
                                                equation=None,          fall-
                                                back_max_timestep=None,
                                                ignore_linear=None,         ig-
                                                nore_independent=None,         ig-
                                                nore_nonlinear=None)
```

Bases: `numericalmodel.numericalschemes.NumericalScheme`

Leap-Frog numerical scheme

step (*time=None, timestep=None, tendency=True*)

```
class numericalmodel.numericalschemes.NumericalScheme (description=None,
                                                         long_description=None,
                                                         equation=None,          fall-
                                                         back_max_timestep=None,
                                                         ignore_linear=None,         ig-
                                                         nore_independent=None,         ig-
                                                         nore_nonlinear=None)
```

Bases: `numericalmodel.utils.ReprObject`, `numericalmodel.utils.LoggerObject`

Base class for numerical schemes

Parameters

- **description** (*str*) – short equation description
- **long_description** (*str*) – long equation description
- **equation** (`DerivativeEquation`) – the equation
- **fallback_max_timestep** (*single numeric*) – the fallback maximum timestep if no timestep can be estimated from the equation

- **ignore_linear** (*bool*) – ignore the linear part of the equation?
- **ignore_independent** (*bool*) – ignore the variable-independent part of the equation?
- **ignore_nonlinear** (*bool*) – ignore the nonlinear part of the equation?

__str__ ()

Stringification

Returns a summary

Return type `str`

_needed_timesteps_for_integration_step (*timestep=None*)

Given a timestep to integrate from now on, what other timesteps of the dependencies are needed?

Parameters **timestep** (*single numeric value*) – the timestep to calculate

Returns the timesteps

Return type `numpy.array`

Note: timestep 0 means the current time

description

The numerical scheme description

Type `str`

equation

The equation the numerical scheme's should solve

Type `DerivativeEquation`

fallback_max_timestep

The numerical scheme's fallback maximum timestep

Type `float`

ignore_independent

Should this numerical scheme ignore the equation's variable-independent addend?

Type `bool`

ignore_linear

Should this numerical scheme ignore the equation's linear factor?

Type `bool`

ignore_nonlinear

Should this numerical scheme ignore the equation's nonlinear addend?

Type `bool`

independent_addend (*time=None*)

Calculate the equation's addend part that is independent of the variable.

Parameters **times** (*single numeric value, optional*) – the time to calculate the derivative. Defaults to the variable's current (last) time.

Returns the independent addend or 0 if `ignore_independent` is True.

Return type `numeric`

integrate (*time=None, until=None*)

Integrate until a certain time, respecting the *max_timestep*.

Parameters

- **time** (*single numeric, optional*) – The time to begin. Defaults to current variable *time*.
- **until** (*single numeric, optional*) – The time to integrate until. Defaults to one *max_timestep* further.

integrate_step (*time=None, timestep=None*)

Integrate “timestep” forward and set results in-place

Parameters

- **time** (*single numeric, optional*) – The time to calculate the step FROM. Defaults to the current variable time.
- **timestep** (*single numeric, optional*) – The timestep to calculate the step. Defaults to *max_timestep*.

linear_factor (*time=None*)

Calculate the equation’s linear factor in front of the variable.

Parameters **times** (*single numeric value, optional*) – the time to calculate the derivative. Defaults to the variable’s current (last) time.

Returns the linear factor or 0 if *ignore_linear* is True.

Return type numeric

long_description

The longer numerical scheme description

Type *str*

max_timestep

Return a maximum timestep for the current state. First tries the *max_timestep_estimate*, then the *fallback_max_timestep*.

Parameters

- **times** (*single numeric value, optional*) – the time to calculate the derivative. Defaults to the variable’s current (last) time.
- **variablevalue** (*np.array, optional*) – the variable value to use. Defaults to the value of self.variable at the given time.

Returns an estimate of the current maximum timestep

Return type *float*

max_timestep_estimate (*time=None, variablevalue=None*)

Based on this numerical scheme and the equation parts, estimate a maximum timestep. Subclasses may override this.

Parameters

- **times** (*single numeric value, optional*) – the time to calculate the derivative. Defaults to the variable’s current (last) time.
- **variablevalue** (*np.array, optional*) – the variable value to use. Defaults to the value of self.variable at the given time.

Returns an estimate of the current maximum timestep. Definitely check the result for integrity.

Return type single numeric or bogus

Raises `Exception` – any exception if something goes wrong

needed_timesteps (*timestep*)

Given a timestep to integrate from now on, what other timesteps of the dependencies are needed?

Parameters **timestep** (*single numeric value*) – the timestep to calculate

Returns the timesteps

Return type `numpy.array`

Note: timestep 0 means the current time

nonlinear_addend (*time=None, variablevalue=None*)

Calculate the derivative's addend part that is nonlinearly dependent of the variable.

Parameters

- **times** (*single numeric value, optional*) – the time to calculate the derivative. Defaults to the variable's current (last) time.
- **variablevalue** (*np.array, optional*) – the variable value to use. Defaults to the value of `self.variable` at the given time.

Returns the nonlinear addend or 0 if `ignore_nonlinear` is `True`.

Return type `res` (numeric)

step (*time, timestep, tendency=True*)

Integrate one “timestep” from “time” forward and return value

Parameters

- **time** (*single numeric*) – The time to calculate the step FROM
- **timestep** (*single numeric*) – The timestep to calculate the step
- **tendency** (*bool, optional*) – return the tendency or the actual value of the variable after the timestep?

Returns The resulting variable value or tendency

Return type `numpy.ndarray`

```
class numericalmodel.numericalschemes.RungeKutta4 (description=None,
                                                    long_description=None,
                                                    equation=None,           fall-
                                                    back_max_timestep=None,
                                                    ignore_linear=None,         ig-
                                                    nore_independent=None,         ig-
                                                    nore_nonlinear=None)
```

Bases: `numericalmodel.numericalschemes.NumericalScheme`

Runte-Kutta-4 numerical scheme

step (*time=None, timestep=None, tendency=True*)

```
class numericalmodel.numericalschemes.SetOfNumericalSchemes (elements=[],      fall-
                                                             back_plan=None)
```

Bases: `numericalmodel.utils.SetOfObjects`

Base class for sets of `NumericalSchemes`

Parameters

- **elements** (*list of NumericalScheme instance*) – the numerical schemes
- **fallback_plan** (*list*) – the fallback plan if automatic planning fails. Depending on the combination of numerical scheme and equations, a certain order of solving the equations is crucial. For some cases, the order can be determined automatically, but if that fails, one has to provide this information by hand. Has to be a list of [*varname*, [*timestep1*, *timestep2*, ...]] pairs.

varname: the name of the equation variable. Obviously there has to be at least one entry in the list for each equation.

timestepN: the normed timesteps (betw. 0 and 1) to calculate. Normed means, that if it is requested to integrate the set of numerical equations by an overall timestep, what percentages of this timestep have to be available of this variable. E.g. an overall timestep of 10 is requested. Another equation needs this variable at the timesteps 2 and 8. Then the timesteps would be [0.2,0.8]. Obviously, the equations that looks farthest into the future (e.g. Runge-Kutta or Euler-Implicit) has to be last in this `fallback_plan` list.

_object_to_key (*obj*)

key transformation function.

Parameters **obj** (*object*) – the element

Returns

the unique key for this object. The equation's variable's `id` is used.

Return type `key` (*str*)

fallback_plan

The fallback plan if automatic plan determination does not work

Type `list`

integrate (*start_time*, *final_time*)

Integrate the model until `final_time`

Parameters

- **start_time** (*float*) – the starting time
- **final_time** (*float*) – time to integrate until

plan

The unified plan for this set of numerical schemes. First try to determine the plan automatically, if that fails, use the `fallback_plan`.

Type `list`

numericalmodel.utils module

class `numericalmodel.utils.LoggerObject` (*logger=<logging.Logger object>*)

Bases: `object`

Simple base class that provides a 'logger' property

Parameters **logger** (*logging.Logger*) – the logger to use

logger

the `logging.Logger` used for logging. Defaults to `logging.getLogger(__name__)`.

class `numericalmodel.utils.ReprObject`

Bases: `object`

Simple base class that defines a `__repr__` method based on an object's `__init__` arguments and properties that are named equally. Subclasses of `ReprObject` should thus make sure to have properties that are named equally as their `__init__` arguments.

`__repr__()`

Python representation of this object

Returns a Python representation of this object based on its `__init__` arguments and corresponding properties.

Return type `str`

classmethod `_full_variable_path(var)`

Get the full string of a variable

Parameters `var` (*any*) – The variable to get the full string from

Returns The full usable variable string including the module

Return type `str`

class `numericalmodel.utils.SetOfObjects` (`elements=[]`, `element_type=<class 'object'>`)

Bases: `numericalmodel.utils.ReprObject`, `numericalmodel.utils.LoggerObject`, `collections.abc.MutableMapping`

Base class for sets of objects

`__str__()`

Stringification

Returns a summary

Return type `str`

`_object_to_key(obj)`

key transformation function. Subclasses should override this.

Parameters `obj` (*object*) – object

Returns the unique key for this object. Defaults to `repr(obj)`

Return type `str`

add_element (`newelement`)

Add an element to the set

Parameters `newelement` (object of type `element_type`) – the new element

element_type

The base type the elements in the set should have

elements

return the list of values

Getter get the list of values

Setter set the list of values. Make sure, every element in the list is an instance of (a subclass of) `element_type`.

Type `list`

`numericalmodel.utils.is_numeric(x)`

Check if a given value is numeric, i.e. whether numeric operations can be done with it.

Parameters **x** (*any*) – the input value

Returns `True` if the value is numeric, `False` otherwise

Return type `bool`

`numericalmodel.utils.utcnow()`

Get the current utc unix timestamp, i.e. the utc seconds since 01.01.1970.

Returns the current utc unix timestamp in seconds

Return type `float`

CHAPTER 7

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