simframe

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CONTENTS:

`simframe` is a Python framework to facilitate scientific simulations. The scope of the software is to provide a framework which can hold data fields, which can be used to integrate differential equations, and which can read and write data files.

Data fields are stored in modified `numpy.ndarrays`. Therefore, `simframe` can only work with data, that can be stored in `NumPy` arrays.

To install `simframe` simply type
`pip install simframe`

Please have a look at the following examples to learn how to use `simframe`.

This notebook teaches how to:
set up frames, create fields, create integration variables, set up derivatives, set up integration instructions, run simulations, write and read data, resume from dump files, and deactivate the progess bar.

In addition to the `simframe` requirements, the following packages are needed for this notebook: `matplotlib`, `scipy`.

CHAPTER

ONE

1. SIMPLE INTEGRATION

In this tutorial we want to solve the most simple differential equation

$\frac{\mathrm{d}Y}{\mathrm{d}x} = b\,Y$

with the initial condition

$Y\,(0) = A.$

This problem has the solution

$Y\,(x) = A\,e^{bx}.$

We set up some parameters that allow us to easily change the problem and rerun the simulation.

[1]:
```
A  = 10.  # Initial value of Y
b  = -1.  # decay factor
dx =  0.1 # Stepsize
```

1.1 Setting up frames

Frame objects are the core functionality of `simframe`. They contain everything you need to run a simulation, from variable to parameters to integration schemes.

[2]:
```
from simframe import Frame
```

Here we set up a `Frame` object called `sim` and give it a meaningful description of our problem.

[3]:
```
sim = Frame(description="Simple Integration")
```

Right now the frame is empty. It contains attributes for integration and writing of data, that we need to specify later.

[4]:
```
sim
```

[4]:
```
Frame (Simple Integration)
--------------------------
    Integrator   : not specified
    Writer       : not specified
```

1.2 Creating fields

We can now fill the empty frame with our problem. First, we create a field for our variable `Y` and initialize it with its initial value `A`. Upon initialization field need to have the correct shape and data type already. This cannot be changed later.

[5]:
```
sim.addfield("Y", A)
```

The frame object has now the field `Y`.

[6]:
```
sim
```

[6]:
```
Frame (Simple Integration)
--------------------------
    Y             : Field
  -----
    Integrator    : not specified
    Writer        : not specified
```

You can do all kinds of operations with `Y` just as with `numpy.ndarray`.

[7]:
```
sim.Y + 3
```

[7]:
```
13.0
```

[8]:
```
import numpy as np
```

[9]:
```
np.exp(sim.Y)
```

[9]:
```
22026.465794806718
```

1.3 Setting up derivatives

To solve for `Y` we have to specify a derivative of the field that can be used by the integrator. The function for the derivative of any variable needs the frame object, the integration variable, and the variable itself as positional arguments and needs to return the value of the derivative.

`derivative(frame, x, Y)`

In our case here the derivative is very simple but more complex equations could also use different fields by adressing them via the `frame` object.

[10]:
```
def dYdx(frame, x, Y):
    return b*Y
```

Now we have to assign this function to the differentiator of our variable `Y`.

[11]:
```
sim.Y.differentiator = dYdx
```

The derivative can be called with `.derivative(x, Y)`. If you don't give `x` or `Y`, then `simframe` assumes the current values, which does not work at this moment, because we have not set `x`, yet.

[12]:
```
sim.Y.derivative(0., A)
```

[12]:
```
-10.0
```

1.4 Creating integration variables

Every frame objects needs at least one integration variable that controls the workflow and is advancing the simulation in space or time for example. In our case this is `x`. Integration variables can be added to the frame object just as fields.

[13]:
```
sim.addintegrationvariable("x", 0.)
```

The frame objects has now the integration variable `x`.

[14]:
```
sim
```

[14]:
```
Frame (Simple Integration)
--------------------------
    x            : IntVar, Integration variable
    Y            : Field
  -----
    Integrator   : not specified
    Writer       : not specified
```

The integration variable is used to advance the simulation in `x` in our case and needs to know about the stesize. We therefore have to create a function that returns `dx`. The only argument of this function has to be the frame object and needs to return the step size.

In our simple case we just want to return a constant step size that we defined earlier.

[15]:
```
def f_dx(frame):
    return dx
```

We now have to tell the updater of the itnegration variable to use this function.

[16]:
```
sim.x.updater = f_dx
```

In addition to that, the integration variable needs to know about snapshots, i.e. points in space or time, when data should be written. Even you don't want to write data, you need to give at least one fineal value, because `simframe` needs to know when to stop the calculation. The snapshots have to be either a list or an array with the desired snapshots in increasing order.

[17]:
```
sim.x.snapshots = np.linspace(1., 10., 10)
```

Compared to regular fields, integration variables have additional functionality. For example we can get the current step size, the maximum possible step size until the next snapshot is written, and the value of the integration variable at the next snapshot.

[18]:
```
sim.x.stepsize
```

[18]:
```
0.1
```

[19]:
```
sim.x.maxstepsize
```

[19]:
```
1.0
```

[20]:
```
sim.x.nextsnapshot
```

[20]:
```
1.0
```

The previously taken stepsize can be accessed with the following attribute, which is set to 0 by default upon initialization.

[21]:
```
sim.x.prevstepsize
```

[21]:
```
0.0
```

1.5 Setting up the integrator

So far we have set up our variables. But we also need to set up an integrator that is performing the actual integration. In our case we want to use a simple explicit Euler 1st-order scheme. The integrator needs the integration variable as positional argument during initialization. We could therefore for example set up different integrators with different integration variables and exchange them midway.

[22]:
```
from simframe import Integrator
```

[23]:
```
sim.integrator = Integrator(sim.x, description="Euler 1st-order")
```

The frame object has now an integrator set.

[24]:
```
sim
```

[24]:
```
Frame (Simple Integration)
--------------------------
    x            : IntVar, Integration variable
    Y            : Field
  -----
    Integrator   : Integrator (Euler 1st-order)
    Writer       : not specified
```

The integrator is basically a container for integration instructions. We therefore have to give tell it which integration instructions it should perform. Instructions have to be a list of `Instruction` objects, which need an integration scheme and a field to be integrated as positional arguments.

[25]:
```
from simframe import Instruction
from simframe import schemes
```

[26]:
```
sim.integrator.instructions = [Instruction(schemes.expl_1_euler, sim.Y)]
```

1.6 Setting up writers

The simulation is now basically ready to go. But in this example we also want to write data files. We therefore have to specify a writer to our frame object. In this case we want to write data files in the `hdf5` format.

[27]:
```
from simframe import writers
```

[28]:
```
sim.writer = writers.hdf5writer()
```

The `hdf5writer` come with a few pre-defined options.

[29]:
```
sim.writer
```

[29]:
```
Writer (HDF5 file format using h5py)
------------------------------------
    Data directory : data
    File names     : data/data0000.hdf5
    Overwrite      : False
    Dumping        : True
    Options        : {'com': 'lzf', 'comopts': None}
    Verbosity      : 1
```

First, we want to change the data directory to which the files are written. If the data directory does not exist, `simframe` will create it.

[30]:
```
sim.writer.datadir = "1_data"
```

And second, we want the writer to overwrite existing files. In that way we can easily restart the notebook with different parameters. Usually a writer will not allow you to overwrite existing files to protect your data.

[31]:
```
sim.writer.overwrite = True
```

[32]:
```
sim.writer
```

[32]:
```
Writer (HDF5 file format using h5py)
------------------------------------
    Data directory : 1_data
    File names     : 1_data/data0000.hdf5
    Overwrite      : True
    Dumping        : True
    Options        : {'com': 'lzf', 'comopts': None}
    Verbosity      : 1
```

By default the writer is writing dump files at every snapshot. In contrast to data files, which only contain the data, a dump file contains the entire frame object from which the simulation can be restarted if anything went wrong. Since these files can be large for bigger projects, it always overwrites the existing dump file.

1.7 Running simulations

The frame objects is now completely set up and we are ready to go.

[33]:
```
sim.run()
```

```
Writing file 1_data/data0000.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0001.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0002.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0003.hdf5
```

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```
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0004.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0005.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0006.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0007.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0008.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0009.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0010.hdf5
Writing dump file 1_data/frame.dmp
Execution time: 0:00:00
```

1.8 Reading data

Every writer should come with a reader that contains instructions for reading the data files the writer has written. It is possible to read a single output file.

[34]:
```
data3 = sim.writer.read.output(3)
```

This returns the namespace containing the data of the chosen output file.

[35]:
```
data3
```

[35]:
```
namespace(Y=array([0.42391158]),
          description=b'Simple Integration',
          x=array([3.]))
```

You can check for existing files in the data directory.

[36]:
```
sim.writer.read.listfiles()
```

[36]:
```
['1_data/data0000.hdf5',
 '1_data/data0001.hdf5',
 '1_data/data0002.hdf5',
 '1_data/data0003.hdf5',
 '1_data/data0004.hdf5',
 '1_data/data0005.hdf5',
 '1_data/data0006.hdf5',
 '1_data/data0007.hdf5',
 '1_data/data0008.hdf5',
 '1_data/data0009.hdf5',
 '1_data/data0010.hdf5']
```

Or you can read the complete data that is in the data directory.

[37]:
```
data = sim.writer.read.all()
```

The fields can be easily adressed just as with the frame object.

[38]:
```
data.Y
```

[38]:
```
array([1.00000000e+01, 3.48678440e+00, 1.21576655e+00, 4.23911583e-01,
       1.47808829e-01, 5.15377521e-02, 1.79701030e-02, 6.26578748e-03,
       2.18474501e-03, 7.61773480e-04, 2.65613989e-04])
```

Instead of reading the full data set or a single snapshots, it is also possible to read a single field from all snapshots.

[39]:
```
seq = sim.writer.read.sequence("x")
```

[40]:
```
seq
```

[40]:
```
array([ 0.,  1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.,  9., 10.])
```

We now want to fit a function to the data to see, if we can reconstruct the initial parameters.

[41]:
```
def fit(x, A, b):
    return A*np.exp(b*x)
```

[42]:
```
from scipy.optimize import curve_fit
```

[43]:
```
popt, pcov = curve_fit(fit, data.x, data.Y)
```

[44]:
```
from IPython.display import Markdown as md
md("| |Simulation|Analytical Solution|\n|:-:|:-:|:-:|\n|A|{:4.2f}|{:4.2f}|\n|b|{:4.2f}|{:
↪4.2f}|".format(popt[0],A,popt[1],b))
```

[44]:

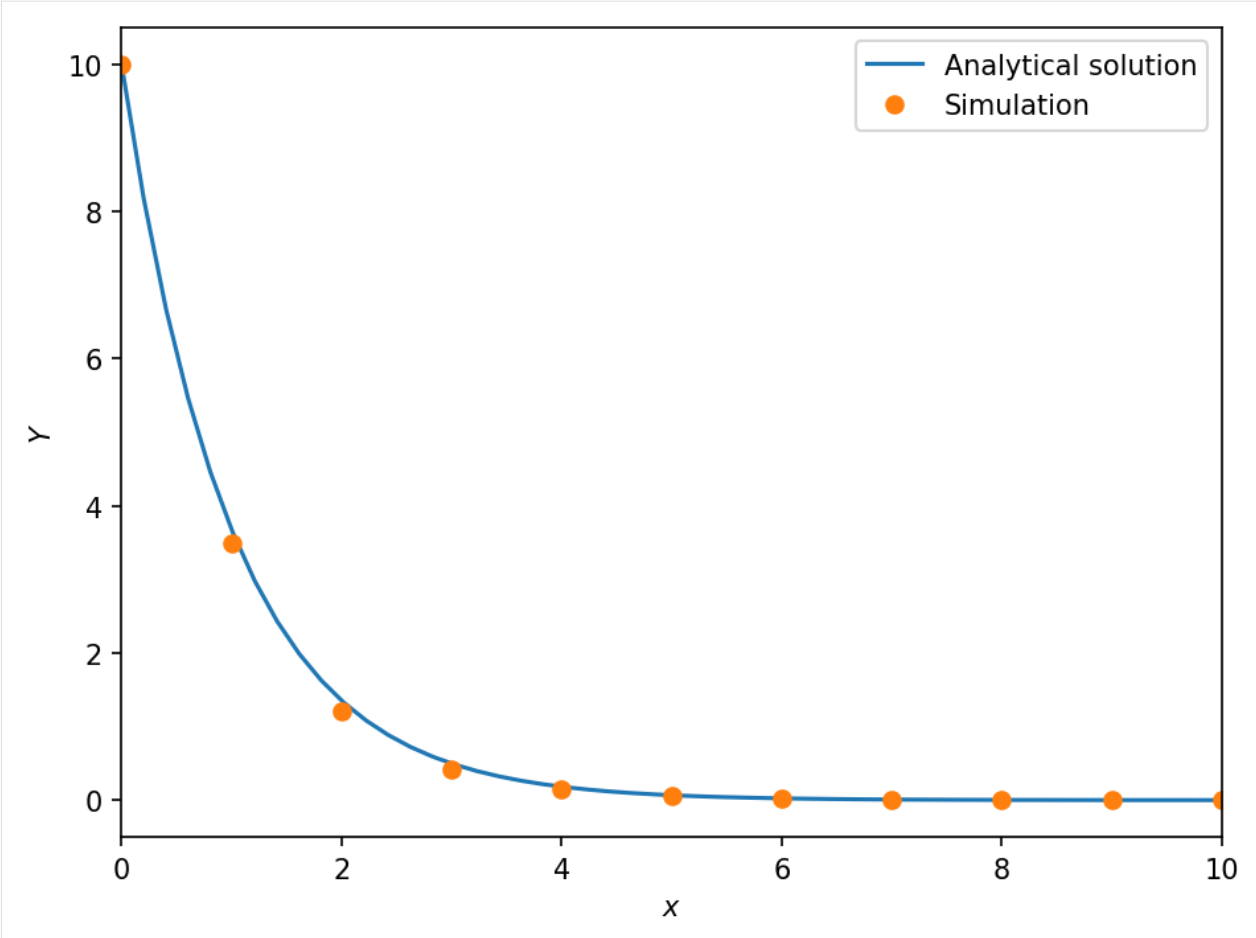
	Simulation	Analytical Solution
A	10.00	10.00
b	-1.05	-1.00

Additionally we want to plot our data.

[45]:
```
import matplotlib.pyplot as plt
```

[46]:
```
def plot(data):
    fig, ax = plt.subplots(dpi=150)
    x = np.linspace(0., 20., 100)
    ax.plot(x, fit(x, A, b), label="Analytical solution")
    ax.plot(data.x, data.Y, "o", label="Simulation")
    ax.set_xlim(data.x[0], data.x[-1])
    ax.set_xlabel("$x$")
    ax.set_ylabel("$Y$")
    ax.legend()
    fig.tight_layout()
    plt.show()
```

[47]:
```
plot(data)
```



1.9 Reading dump files

Let's say we want to continue the simulation from a dump file that we have stored somewhere. We first have to read the file with `readdump(filename)` which needs the path to the file as argument and which returns a frame object.

[48]:
```
from simframe.io import readdump
```

[49]:
```
sim_cont = readdump("1_data/frame.dmp")
```

[50]:
```
sim_cont
```

[50]:
```
Frame (Simple Integration)
--------------------------
    x            : IntVar, Integration variable
    Y            : Field
  -----
    Integrator   : Integrator (Euler 1st-order)
    Writer       : Writer (HDF5 file format using h5py)
```

We only have to add a few more snapshots.

[51]:
```
sim_cont.x.snapshots = np.linspace(1., 20., 20)
```

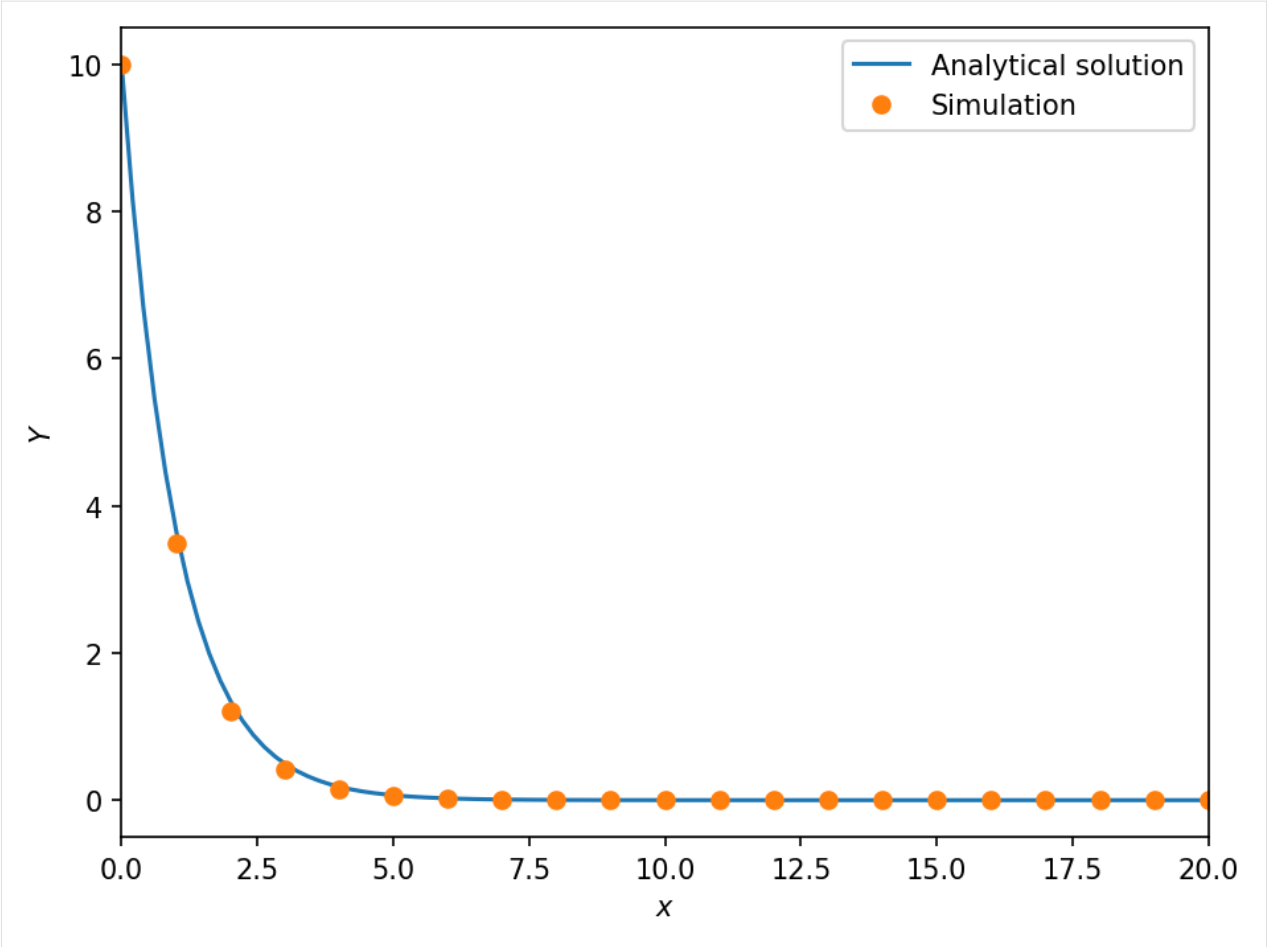
Now we can restart the simulation from the current state, read the data, and plot it.

[52]:
```
sim_cont.run()
```

```
Writing file 1_data/data0011.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0012.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0013.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0014.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0015.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0016.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0017.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0018.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0019.hdf5
Writing dump file 1_data/frame.dmp
Writing file 1_data/data0020.hdf5
Writing dump file 1_data/frame.dmp
Execution time: 0:00:00
```

[53]:
```
data = sim_cont.writer.read.all()
```

[54]:
```
plot(data)
```



1.10 Progress bar

If you are running `simframe` on an interactive shell if will show by default a progress bar with an estimate of the expected computation time. If you want to turn it off to save some computational overhead you can do so by reducing the verbosity of the frame object.

[55]:
```
sim.verbosity = 0
```

This notebook teaches how to:
create groups, create immutable fields, display the table of contents, and set up complex integration instructions.

CHAPTER

TWO

2. ADVANCED INTEGRATION

Let's have a look at orbital integration.
Consider a planet Earth orbiting the Sun. How does its orbit look like?

The equations of motion are determined by a set of two differential equations for the position $\vec{r}$ and velocity $\vec{v}$ of Earth and Sun..

$\frac{\mathrm{d}}{\mathrm{d}t}\vec{r} = \vec{v}$

$m\frac{\mathrm{d}}{\mathrm{d}t}\vec{v} = \vec{F}_\mathrm{G}$

The gravitational force F_G of a body of mass M and position $\vec{R}$ acting on a body of mass m at position $\vec{r}$ is given by

$\vec{F}_\mathrm{G} = -GmM\frac{\vec{r}-\vec{R}}{|\vec{r}-\vec{R}|^3}$

2.1 Creating groups

First we need to add fields for postion, velocity, and mass for Earth and Sun.
To have more structure we group the fields by Earth and Sun. This can be done with `addgroup(name)`.

[1]:
```
from simframe import Frame
```

[2]:
```
sim = Frame(description="Earth-Sun system")
```

[3]:
```
sim.addgroup("Sun")
sim.addgroup("Earth")
```

The frame object has now two groups for Earth and Sun, that can be adressed just as fields.

[4]:
```
sim
```

[4]:
```
Frame (Earth-Sun system)
------------------------
    Earth         : Group
    Sun           : Group
  -----
    Integrator    : not specified
    Writer        : not specified
```

We will keep the problem general in three dimensions, but we will only use two of them for simplicity.
Although spherical coordinates would be more suitable for the problem, we will use Carteesian coordinates here.

First, we need to define a few constants.

[5]:
```
AU      = 1.495978707e11        # Astronomical unit [m]
day     = 8.64e4                # Day [s]
G       = 6.6743e-11            # Gravitational constant [m^3/kg/s^2]
year    = 3.15576e7             # Year [s]

M_earth = 5.972167867791379e24  # Mass of the Earth [kg]
M_sun   = 1.988409870698051e30  # Mass of the Sun [kg]
```

2.2 Creating immutable fields

We can now fill the groups with the variables we need, starting with the masses.
Again: the initial values must have the correct shape and data types.

[6]:
```
sim.Earth.addfield("M", M_earth, description="Mass [kg]")
```

The groups and the fields within can be easily accessed with

[7]:
```
sim.Earth
```

[7]:
```
Group
-----
    M            : Field (Mass [kg])
  -----
```

[8]:
```
sim.Earth.M
```

[8]:
```
5.972167867791379e+24
```

The mass of the Earth shall be constant throughout the simulation. We therefore set a flag so we cannot accidentally change its value.

[9]:
```
sim.Earth.M.constant = True
```

[10]:
```
sim.Earth
```

[10]:
```
Group
-----
    M            : Field (Mass [kg]), constant
  -----
```

Now we add the mass of the Sun, which we directly set to constant when adding the field.

[11]:
```
sim.Sun.addfield("M", M_sun, constant=True, description="Mass [kg]")
```

[12]:
```
sim.Sun
```

[12]:
```
Group
-----
    M            : Field (Mass [kg]), constant
  -----
```

We can do all sorts of operations with those fields, such as calculating the mass ratio.

[13]:
```
sim.Earth.M / sim.Sun.M
```

[13]:
```
3.0034893488507934e-06
```

Now we need to add fields for position and velocity. We initialize them with zeros and think later about the initial conditions.
The important thing is that the have the right shape upon initialization.

[14]:
```
import numpy as np
```

[15]:
```
sim.Earth.addfield("r", np.zeros(3), description="Position [m]")
sim.Earth.addfield("v", np.zeros(3), description="Velocity [m/s]")
sim.Sun.addfield("r", np.zeros(3), description="Position [m]")
sim.Sun.addfield("v", np.zeros(3), description="Velocity [m/s]")
```

[16]:
```
sim.Earth
```

[16]:
```
Group
-----
    M            : Field (Mass [kg]), constant
    r            : Field (Position [m])
    v            : Field (Velocity [m/s])
  -----
```

[17]:
```
sim.Sun
```

[17]:
```
Group
-----
    M            : Field (Mass [kg]), constant
    r            : Field (Position [m])
    v            : Field (Velocity [m/s])
  -----
```

Setting the integration variable

For our simulation we need an integration variable. In our case this is the time.

[18]:
```
sim.addintegrationvariable("t", 0., description="Time [s]")
```

We'll set the step size to a constant value of one day.

[19]:
```
dt = 1.*day
```

[20]:
```
def f_dt(frame):
    return dt
```

[21]:
```
sim.t.updater = f_dt
```

We want to integrate for two years and want to have a snapshot every ten days.

[22]:
```
snapwidth = 10.*day
tmax = 2.*year
```

[23]:
```
sim.t.snapshots = np.arange(snapwidth, tmax, snapwidth)
```

Note: If the initial value of the integration variable is smaller the first snapshot, `simframe` automatically writes an output with initial conditions, if a writer is set.

[24]:
```
sim
```

[24]:
```
Frame (Earth-Sun system)
------------------------
    Earth        : Group
    Sun          : Group
  -----
    t            : IntVar (Time [s]), Integration variable
  -----
    Integrator   : not specified
    Writer       : not specified
```

Setting the writer

As a writer we use the namespacewriter, which does not write the data into files, but stores them within a buffer in the writer.

[25]:
```
from simframe import writers
```

[26]:
```
sim.writer = writers.namespacewriter()
```

The namespacewriter is by default not writing dump files.

[27]:
```
sim.writer
```

[27]:
```
Writer (Temporary namespace writer)
-----------------------------------
    Data directory : data
    Dumping        : False
    Verbosity      : 1
```

Adding differential equations

As a next step we'll add differential equations to the quantities. The differential equations for the positions are simple. We simply return the velocities, which we can adress with the `frame` argument.

[28]:
```
def dr_Earth(frame, x, Y):
    return frame.Earth.v
```

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```
def dr_Sun(frame, x, Y):
    return frame.Sun.v
```

For the differential equations of the velocities we'll write a little helper function that computes the gravitational accelleration.

[29]:
```
# Gravitational acceleration
def ag(M, r, R):
    direction = r-R
    distance = np.linalg.norm(direction)
    return -G * M * direction / distance**3
```

[30]:
```
def dv_Earth(frame, x, Y):
    return ag(frame.Sun.M, frame.Earth.r, frame.Sun.r)

def dv_Sun(frame, x, Y):
    return ag(frame.Earth.M, frame.Sun.r, frame.Earth.r)
```

Now we need to add the differential equations to their fields.

[31]:
```
sim.Earth.v.differentiator = dv_Earth
sim.Earth.r.differentiator = dr_Earth
sim.Sun.v.differentiator   = dv_Sun
sim.Sun.r.differentiator   = dr_Sun
```

2.3 Displaying the table of contents

You can also display the complete tree structure of your frame.

[32]:
```
sim.toc
```

```
Frame (Earth-Sun system)
    - Earth: Group
        - M: Field (Mass [kg]), constant
        - r: Field (Position [m])
        - v: Field (Velocity [m/s])
    - Sun: Group
        - M: Field (Mass [kg]), constant
        - r: Field (Position [m])
        - v: Field (Velocity [m/s])
    - t: IntVar (Time [s]), Integration variable
```

2.4 Inspecting memory usage

It is possible to print out the memory usage in bytes of a group with the command

[33]:
```
sim.memory_usage()
```

[33]:
```
341.0
```

Further details can be displayed with the keyword argument `print_output`, while `skip_hidden` will ommit attributes starting with underscore _:

[34]:
```
sim.memory_usage(print_output=True, skip_hidden=True)
```

```
    - Earth:                                    total:  56   B
        - M:                                      (1,)   8   B
        - r:                                      (3,)  24   B
        - v:                                      (3,)  24   B
    - Sun:                                      total:  56   B
        - M:                                      (1,)   8   B
        - r:                                      (3,)  24   B
        - v:                                      (3,)  24   B
    - t:                                          (1,)   8   B

Total: 120   B
```

[34]:
```
120.0
```

2.5 Setting up complex integration instructions

Next we need to set up the integrator. We integrate all quantities with the explicit Euler 1st-order scheme as in the previous tutorial, but this time he have to integrate four fields. This can be easily achieved by adding four instructions.

[35]:
```
from simframe import Integrator
from simframe.integration import Instruction
from simframe import schemes
```

[36]:
```
sim.integrator = Integrator(sim.t, description="Euler 1st-order")
```

[37]:
```
instructions_euler = [Instruction(schemes.expl_1_euler, sim.Earth.r),
                      Instruction(schemes.expl_1_euler, sim.Earth.v),
                      Instruction(schemes.expl_1_euler, sim.Sun.r  ),
                      Instruction(schemes.expl_1_euler, sim.Sun.v  ),
                     ]
```

[38]:
```
sim.integrator.instructions = instructions_euler
```

Initial conditions

Before we can start the simulation, we have to think about initial conditions.

If we simply set the Sun at rest in the center of our simulation and only set the position and velocity of the Earth, then the center of mass would have a non-zero momentum and would slowly drift away from its initial position.

So what we do first: we set the Sun's positon to zero (i.e., don't do anything) and the Earth's position to a distance of 1 AU in positive x-direction. Then we'll offset their positions to center the system on the center of mass instead onto the Sun.

[39]:
```
r_Earth_ini = np.array([AU, 0., 0.])
r_Sun_ini = np.zeros(3)
# Center of mass
COM_ini = (M_earth*r_Earth_ini + M_sun*r_Sun_ini) / (M_earth+M_sun)
# Offset both positions
r_Earth_ini -= COM_ini
r_Sun_ini -= COM_ini
```

We save them in a separate variable instead of assigning them directly for later use.

The inital orbital velocities of the Earth shall be in positive y-direction, the velocity of the Sun in negative y-direction. For calculating the value we use the reduced mass mu of the system.

[40]:
```
mu = M_earth*M_sun / (M_earth+M_sun)
```

[41]:
```
v_Earth_ini = np.array([0., np.sqrt(G*M_sun/M_earth*mu/AU), 0.])
v_Sun_ini   = np.array([0., -np.sqrt(G*M_earth/M_sun*mu/AU), 0.])
```

Now we assign them to their fields.

[42]:
```
sim.Earth.r = r_Earth_ini
sim.Earth.v = v_Earth_ini
sim.Sun.r   = r_Sun_ini
sim.Sun.v   = v_Sun_ini
```

Starting the simulation

[43]:
```
sim.run()
```

```
Saving frame 0000
Saving frame 0001
Saving frame 0002
Saving frame 0003
Saving frame 0004
Saving frame 0005
Saving frame 0006
Saving frame 0007
Saving frame 0008
Saving frame 0009
Saving frame 0010
Saving frame 0011
Saving frame 0012
Saving frame 0013
Saving frame 0014
Saving frame 0015
Saving frame 0016
Saving frame 0017
Saving frame 0018
```

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```
Saving frame 0019
Saving frame 0020
Saving frame 0021
Saving frame 0022
Saving frame 0023
Saving frame 0024
Saving frame 0025
Saving frame 0026
Saving frame 0027
Saving frame 0028
Saving frame 0029
Saving frame 0030
Saving frame 0031
Saving frame 0032
Saving frame 0033
Saving frame 0034
Saving frame 0035
Saving frame 0036
Saving frame 0037
Saving frame 0038
Saving frame 0039
Saving frame 0040
Saving frame 0041
Saving frame 0042
Saving frame 0043
Saving frame 0044
Saving frame 0045
Saving frame 0046
Saving frame 0047
Saving frame 0048
Saving frame 0049
Saving frame 0050
Saving frame 0051
Saving frame 0052
Saving frame 0053
Saving frame 0054
Saving frame 0055
Saving frame 0056
Saving frame 0057
Saving frame 0058
Saving frame 0059
Saving frame 0060
Saving frame 0061
Saving frame 0062
Saving frame 0063
Saving frame 0064
Saving frame 0065
Saving frame 0066
Saving frame 0067
Saving frame 0068
Saving frame 0069
Saving frame 0070
```

(continues on next page)

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```
Saving frame 0071
Saving frame 0072
Saving frame 0073
Execution time: 0:00:00
```

Reading and plotting

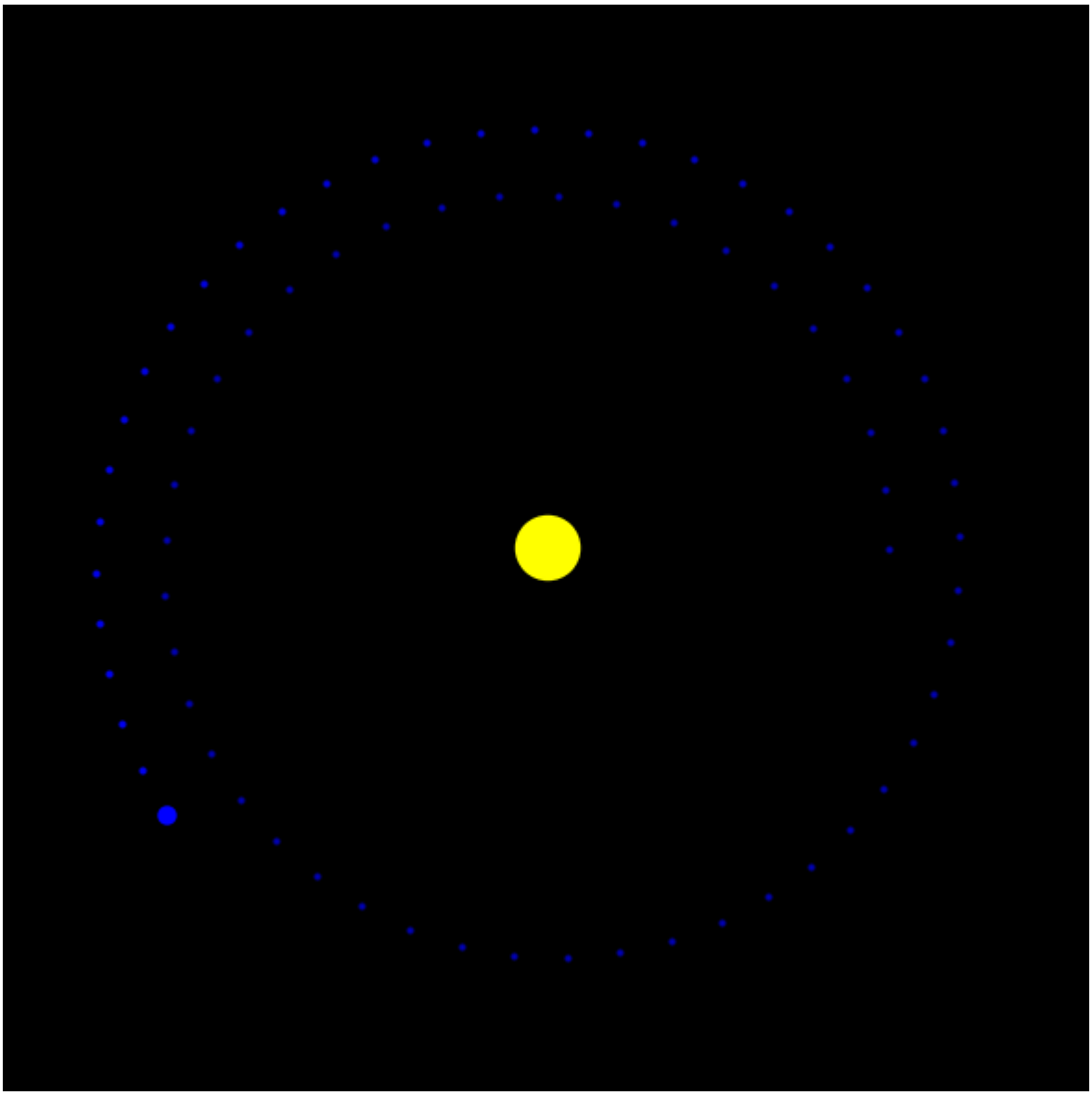
Reading data from the namespace writer works identical to the writer discussed earlier.

[44]:
```
data_euler = sim.writer.read.all()
```

[45]:
```
import matplotlib.pyplot as plt

def plot_orbits(data):
    fig, ax = plt.subplots(dpi=150)
    ax.set_aspect(1)
    ax.axis("off")
    fig.set_facecolor("#000000")
    imax = data.t.shape[0]
    for i in range(imax):
        alpha = np.maximum(i/imax-0.1, 0.5)
        ax.plot(data.Sun.r[i, 0], data.Sun.r[i, 1], "o", c="#FFFF00", markersize=4,␣
↪alpha=alpha)
        ax.plot(data.Earth.r[i, 0], data.Earth.r[i, 1], "o", c="#0000FF", markersize=1,␣
↪alpha=alpha)
    ax.plot(data.Sun.r[-1, 0], data.Sun.r[-1, 1], "o", c="#FFFF00", markersize=16)
    ax.plot(data.Earth.r[-1, 0], data.Earth.r[-1, 1], "o", c="#0000FF", markersize=4)
    ax.set_xlim(-1.5*AU, 1.5*AU)
    ax.set_ylim(-1.5*AU, 1.5*AU)
    fig.tight_layout()
    plt.show()
```

[46]:
```
plot_orbits(data_euler)
```



2.6 Leapfrog integration

As you can see, the Earth is not on a circular orbit. Its orbital distance is increasing and because of that the Earth could not achieve two full orbital cycles.

The problem is the simple integration scheme used here.
Every integration scheme has numerical error. Some have larger ones than others. Euler's 1st order method is simply not suited for orbital integration.

But there is a way out: Symplectic integration
Symplectic integrators conserve the energy of the system.

One of these methods is the Leapfrog method.

Leapfrogging means the velocity and the position are not updated synchronous, but in between each other. They are leapfroggin each other.

In our case we first update the velocities by using half of the step size. Then we update the positions for a full time step. And finally, we update the velocities for another semi time step. We can do this by using the `fstep` keyword argument for the instructions, which is the fraction of the time for which this instruction is applied.

But there is one caveat: usually the fields that are integrated in an instructions set are only updated after all instructions have been executed, such that the second instruction still sees the original value of the first variable and not already the new value.

But for leapfrog integration, the instruction for the positions already need to know the new values of the velocities. And the second set of velocity instructions already need to know the new positions. We therefore have to add `update` instructions in between.

We do not have to add update instructions after the second set of velocity operations, because at the end of an instruction set all fields contained in the instruction set will be updated.

The new leapfrog instruction set now looks like this.

[47]:
```
instructions_leapfrog = [Instruction(schemes.expl_1_euler, sim.Sun.v,   fstep=0.5),
                         Instruction(schemes.expl_1_euler, sim.Earth.v, fstep=0.5),
                         Instruction(schemes.update,       sim.Sun.v            ),
                         Instruction(schemes.update,       sim.Earth.v          ),
                         Instruction(schemes.expl_1_euler, sim.Sun.r,   fstep=1.0),
                         Instruction(schemes.expl_1_euler, sim.Earth.r, fstep=1.0),
                         Instruction(schemes.update,       sim.Sun.r            ),
                         Instruction(schemes.update,       sim.Earth.r          ),
                         Instruction(schemes.expl_1_euler, sim.Sun.v,   fstep=0.5),
                         Instruction(schemes.expl_1_euler, sim.Earth.v, fstep=0.5),
                        ]
```

We can assign this new instruction set to our frame. To rerun the simulation we have to reset the initial conditions, that we've saved earlier.

[48]:
```
sim.integrator.instructions = instructions_leapfrog
sim.integrator.description = "Leapfrog integrator"
sim.Earth.r = r_Earth_ini
sim.Earth.v = v_Earth_ini
sim.Sun.r   = r_Sun_ini
sim.Sun.v   = v_Sun_ini
sim.t       = 0.
```

Additionally we have to reset the buffer of the namespace writer. Otherwise, we would simply add snapshots to the old dataset. Furthermore, we descrease the `verbosity` of the writer to prevent it from writing information on screen.

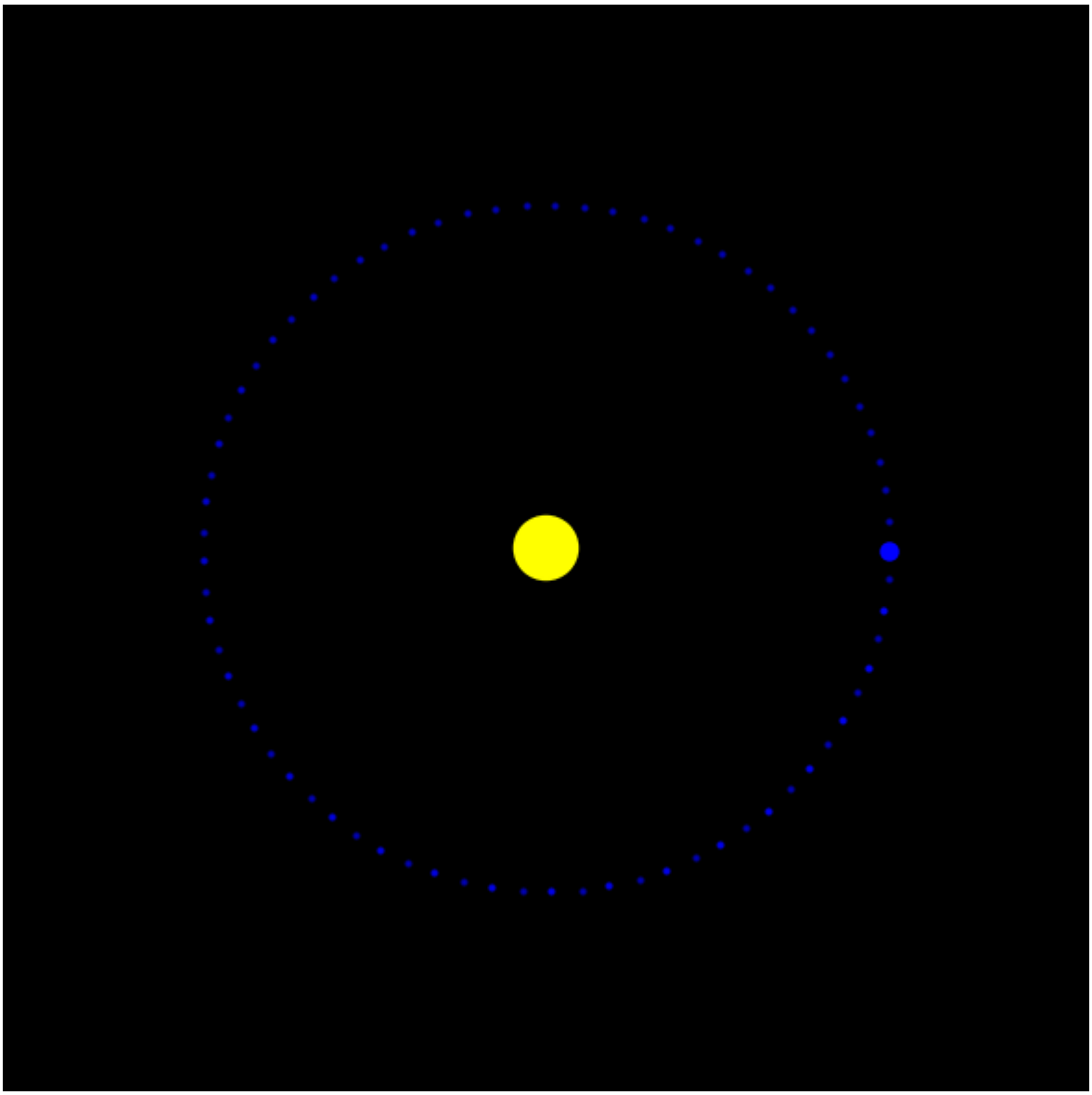
[49]:
```
sim.writer.reset()
sim.writer.verbosity = 0
```

[50]:
```
sim.run()
```

```
Execution time: 0:00:00
```

[51]:
```
data_leapfrog = sim.writer.read.all()
```

[52]:
```
plot_orbits(data_leapfrog)
```



This notebook teaches how to:
update groups and fields and use heartbeats.

In addition to the `simframe` requirements, the following packages are needed for this notebook: `astropy`, `matplotlib`.

CHAPTER

THREE

3. UPDATING GROUPS AND FIELDS

In this example we revisit the orbital integration from the previous tutorial. But this time we also want to calculate the equilibrium temperature on Earth. That is not a quantity that we need to integrate. We can simply calculate it from the other quantities. But we have to tell `simframe` how to do it.

Setting up the problem

The problem setup follows the previous example. Please have a look there for more details.

[1]:
```
from simframe import Frame
```

[2]:
```
sim = Frame(description="Earth-Sun system")
```

[3]:
```
sim.addgroup("Sun")
sim.addgroup("Earth")
```

[4]:
```
import astropy.constants as c
import astropy.units as u
```

[5]:
```
AU   = (1.*u.au).si.value
day  = (1.*u.day).si.value
G    = c.G.si.value
year = (1.*u.year).si.value

M_earth = c.M_earth.si.value
M_sun   = c.M_sun.si.value
```

Earth

[6]:
```
import numpy as np
```

[7]:
```
sim.Earth.addfield("M", M_earth, description="Mass [kg]", constant=True)
sim.Earth.addfield("r", np.zeros(3), description="Position [m]")
sim.Earth.addfield("v", np.zeros(3), description="Velocity [m/s]")
```

Sun

[8]:
```
sim.Sun.addfield("M", c.M_sun.si.value, description="Mass [kg]", constant=True)
sim.Sun.addfield("r", np.zeros(3), description="Position [m]")
sim.Sun.addfield("v", np.zeros(3), description="Velocity [m/s]")
```

Integration variable

[9]:
```
sim.addintegrationvariable("t", 0., description="Time [s]")
```

[10]:
```
dt = 1.*day
```

[11]:
```
def f_dt(frame):
    return dt
```

[12]:
```
sim.t.updater = f_dt
```

[13]:
```
snapwidth = 5.*day
tmax = 2.*year
```

[14]:
```
sim.t.snapshots = np.arange(snapwidth, tmax+1, snapwidth)
```

Writer

[15]:
```
from simframe import writers
```

[16]:
```
sim.writer = writers.namespacewriter()
```

[17]:
```
sim.writer.verbosity = 0
```

Differential equations

[18]:
```
def dr_Earth(frame, x, Y):
    return frame.Earth.v

def dr_Sun(frame, x, Y):
    return frame.Sun.v
```

[19]:
```
# Gravitational acceleration
def ag(M, r, R):
    direction = r-R
    distance = np.linalg.norm(direction)
    return -G * M * direction / distance**3
```

[20]:
```
def dv_Earth(frame, x, Y):
    return ag(frame.Sun.M, frame.Earth.r, frame.Sun.r)

def dv_Sun(frame, x, Y):
    return ag(frame.Earth.M, frame.Sun.r, frame.Earth.r)
```

[21]:
```
sim.Earth.v.differentiator = dv_Earth
sim.Earth.r.differentiator = dr_Earth
sim.Sun.v.differentiator   = dv_Sun
sim.Sun.r.differentiator   = dr_Sun
```

Integrator

[22]:
```
from simframe import Integrator
```

[23]:
```
integrator = Integrator(sim.t, description="Leapfrog integratior")
```

[24]:
```
from simframe import schemes
from simframe.integration import Instruction
```

Leapfrog integrator

[25]:
```
instructions = [Instruction(schemes.expl_1_euler, sim.Sun.v,   fstep=0.5),
                Instruction(schemes.expl_1_euler, sim.Earth.v, fstep=0.5),
                Instruction(schemes.update,       sim.Sun.v            ),
                Instruction(schemes.update,       sim.Earth.v          ),
                Instruction(schemes.expl_1_euler, sim.Sun.r,   fstep=1.0),
                Instruction(schemes.expl_1_euler, sim.Earth.r, fstep=1.0),
                Instruction(schemes.update,       sim.Sun.r            ),
                Instruction(schemes.update,       sim.Earth.r          ),
                Instruction(schemes.expl_1_euler, sim.Sun.v,   fstep=0.5),
                Instruction(schemes.expl_1_euler, sim.Earth.v, fstep=0.5),
               ]
```

[26]:
```
integrator.instructions = instructions
```

[27]:
```
sim.integrator = integrator
```

Initial conditions

In this example we want to send the Earth on an eccentric orbit to have a seasonal change in the equilibrium temperature. For this we simply incline the initial velocities of Earth an Sun by an angle `alpha`.

[28]:
```
r_Earth_ini = np.array([AU, 0., 0.])
r_Sun_ini = np.zeros(3)
# Center of mass
COM_ini = (M_earth*r_Earth_ini + M_sun*r_Sun_ini) / (M_earth+M_sun)
# Offset both positions
r_Earth_ini -= COM_ini
r_Sun_ini -= COM_ini
```

[29]:
```
mu = M_earth*M_sun / (M_earth+M_sun)
```

[30]:
```
alpha = 30. * u.deg
v_Earth_ini = np.sqrt(G*M_sun/M_earth*mu/AU)
v_Earth_ini = np.array([-np.sin(alpha)*v_Earth_ini, np.cos(alpha)*v_Earth_ini, 0.])
v_Sun_ini   = np.sqrt(G*M_earth/M_sun*mu/AU)
v_Sun_ini   = np.array([np.sin(alpha)*v_Sun_ini, -np.cos(alpha)*v_Sun_ini, 0.])
```

[31]:
```
sim.Earth.r = r_Earth_ini
sim.Earth.v = v_Earth_ini
sim.Sun.r   = r_Sun_ini
sim.Sun.v   = v_Sun_ini
```

Starting

[32]:
```
sim.run()
```

```
Execution time: 0:00:00
```

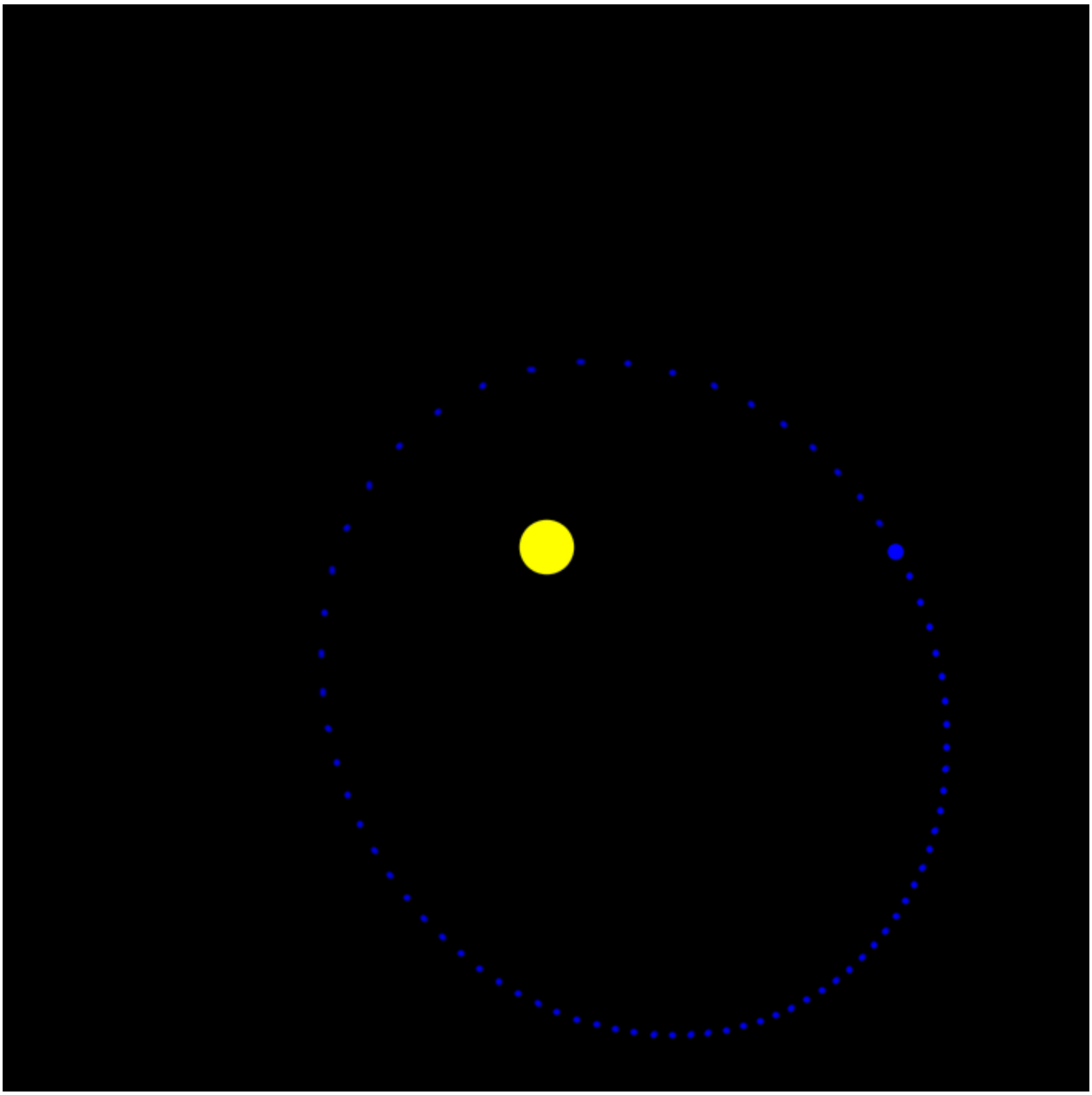
Reading and plotting

[33]:
```
data = sim.writer.read.all()
```

[34]:
```
import matplotlib.pyplot as plt

def plot_orbits(data):
    fig, ax = plt.subplots(dpi=150)
    ax.set_aspect(1)
    ax.axis("off")
    fig.set_facecolor("#000000")
    imax = data.t.shape[0]
    for i in range(imax):
        alpha = np.maximum(i/imax-0.1, 0.5)
        ax.plot(data.Sun.r[i, 0], data.Sun.r[i, 1], "o", c="#FFFF00", markersize=4,␣
↪alpha=alpha)
        ax.plot(data.Earth.r[i, 0], data.Earth.r[i, 1], "o", c="#0000FF", markersize=1,␣
↪alpha=alpha)
    ax.plot(data.Sun.r[-1, 0], data.Sun.r[-1, 1], "o", c="#FFFF00", markersize=16)
    ax.plot(data.Earth.r[-1, 0], data.Earth.r[-1, 1], "o", c="#0000FF", markersize=4)
    ax.set_xlim(-1.5*AU, 1.5*AU)
    ax.set_ylim(-1.5*AU, 1.5*AU)
    fig.tight_layout()
    plt.show()
```

[35]:
```
plot_orbits(data)
```



The Earth is now on an eccentric orbit around the sound. By the spacing of the snapshots, which are constant in time, you can even tell that the Earth is faster around the perihelion and slower around the aphelion.

Adding Temperature

To calculate the temperature Earth and Sun need additional fields for their temperatures and their radii. In additional to that, we give the Earth an additional field for the Earth-Sun distance.

[36]:
```
R_Earth = c.R_earth.si.value
R_Sun   = c.R_sun.si.value
```

We initialize the Earth's temperature with zero and update it as soon as we have a function for it.

[37]:
```
sim.Earth.addfield("d", AU, description="Earth-Sun distance [m]")
sim.Earth.addfield("R", R_Earth, description="Radius [m]")
sim.Earth.addfield("T", 0., description="Temperature [K]")
```

[38]:
```
sim.Earth
```

[38]:
```
Group
-----
    d            : Field (Earth-Sun distance [m])
    M            : Field (Mass [kg]), constant
    r            : Field (Position [m])
    R            : Field (Radius [m])
    T            : Field (Temperature [K])
    v            : Field (Velocity [m/s])
  -----
```

[39]:
```
sim.Sun.addfield("R", R_Sun, description="Radius [m]", constant=True)
sim.Sun.addfield("T", 5778, description="Effective temperature [K]", constant=True)
```

[40]:
```
sim.Sun
```

[40]:
```
Group
-----
    M            : Field (Mass [kg]), constant
    r            : Field (Position [m])
    R            : Field (Radius [m]), constant
    T            : Field (Effective temperature [K]), constant
    v            : Field (Velocity [m/s])
  -----
```

3.1 Skipping Fields in Output Files

It is possible to not write certain fields into the output. This can be especially useful if you have large fields, that consume a significant amount of memory, that you don't need for your data analysis. Simply the the `save` attribute to `False`.

[41]:
```
sim.Sun.T.save = False
```

3.2 Updating fields

The energy the sun is emitting per time, i.e., it's luminosity L, is given by

$L_\odot = 4\pi R_\odot^2 \sigma_{\rm SB} T_{\rm eff}^4$.

The energy flux arriving at Earth, i.e., the Solar constant S is then given by

$S = \frac{L}{4\pi d^2}$.

Only one hemisphere of the Earth is illuminated at any time, so the energy that the Earth is receiving per unit time, neglecting any albedo effects, is given by

$P_{\rm in} = \pi R_\oplus^2 S$.

We assume that the temperature on Earth is in euilibrium, i.e., there is no difference between day and night. The energy the Earth is emitting per unit time is then given by

$P_{\mathrm{out}} = 4\pi R_{\oplus}^2 \sigma_{\mathrm{SB}} T^4$.

In equilibrium both are equal ($P_{\mathrm{in}} = P_{\mathrm{out}}$) and we can solve for T

$T = T_{\mathrm{eff}} \sqrt[4]{\frac{R_{\odot}^2}{4d^2}}$.

So the equilibrium temperature on Earth depends on the Sun's effective temperature T_{eff}, the Sun's radius $R_{\odot}$, and the Earth-Sun distance d. We can now write a function that takes the frame object as argument and returns Earth's temperature.

[42]:
```
sigma_sb = c.sigma_sb.si.value
```

[43]:
```
def T(frame):
    """Function computes the equilibrium temperature of the Earth"""
    return frame.Sun.T * (frame.Sun.R**2 / (4.*frame.Earth.d**2))**0.25
```

We can now assign this function to the updater of the temperature field

[44]:
```
sim.Earth.T.updater = T
```

The function for calculating the Earth-Sun distance is pretty simple and can be simply assigned to the updater of the field.

[45]:
```
def d(sim):
    """Function computed the Sun-Earth distance"""
    return np.linalg.norm(sim.Earth.r - sim.Sun.r)
```

[46]:
```
sim.Earth.d.updater = d
```

Right now the temperature is zero as we initialized it.

[47]:
```
sim.Earth.T
```

[47]:
```
0.0
```

We can now use our the updater of the temperature field to calculate it's initial value

[48]:
```
sim.Earth.T.update()
```

[49]:
```
sim.Earth.T
```

[49]:
```
278.6190681198289
```

3.3 Updating groups

But before we can rerun the simulation we have to tell `simframe` how to update groups. This is not done automatically, because for one, not all fields and groups need to be updated, and second, the order of update matters. In our case, we do not need to update the group of the Sun, because it's temperature is not changing, and we need to update the Earth-Sun distance before we update the Earth's temperature, because we need the distance for it.

The only update operation that is performed once per time step is the update of the frame object `Frame.update()`. From here we have to delegate tasks down the tree structure.

There are in principle two methods of updating groups. One is by writing a function and assigning it to the group's updater. Here we write a function that is calling Earth's updater and assign it to theupdater of the frame.

[50]:
```
def update_Earth(frame):
    frame.Earth.update()
```

[51]:
```
sim.updater = update_Earth
```

The second method is by assigning a list of group attributes to an updater. The updater is then calling the updaters of these attributes in exactly that order.

[52]:
```
sim.Earth.updater = ["d", "T"]    # Earth-Sun distance first, then temperature
```

If the updater of a group has been set with a list, the order can be displayed. The attribute will return `None`, if no updater is set or if the updater was set with a function.

[53]:
```
sim.Earth.updateorder
```

[53]:
```
['d', 'T']
```

Resetting to initial conditions

We can now reset to the initial conditions we have saved earlier, reset the namespace writer, and run the simulation again.

[54]:
```
sim.Earth.r = r_Earth_ini
sim.Earth.v = v_Earth_ini
sim.Sun.r   = r_Sun_ini
sim.Sun.v   = v_Sun_ini
sim.t       = 0.
sim.writer.reset()
```

[55]:
```
sim.run()
```

```
Execution time: 0:00:00
```

Reading and plotting

[56]:
```
data_T = sim.writer.read.all()
```

[57]:
```
def plot_temperature(data):
    fig, ax = plt.subplots(dpi=150)
    ax.plot(data.t/year, (data.Earth.T*u.K).to(u.Celsius, equivalencies=u.temperature()),
↪ c="C3", label="Temperature")
    ax.plot(-2., 0., label="Earth-Sun distance", c="C0")
    ax.set_xlabel("Time [years]")
    ax.set_ylabel("Temperature [°C]")
    ax.set_xlim(data.t[0]/year, data.t[-1]/year)
    ax.set_ylim(-100., 150.)
    axr = ax.twinx()
    axr.plot(data.t/year, data.Earth.d/AU, c="C0")
    axr.set_ylabel("Distance [AU]")
    axr.set_ylim(0., 2.0)
    ax.legend()
```

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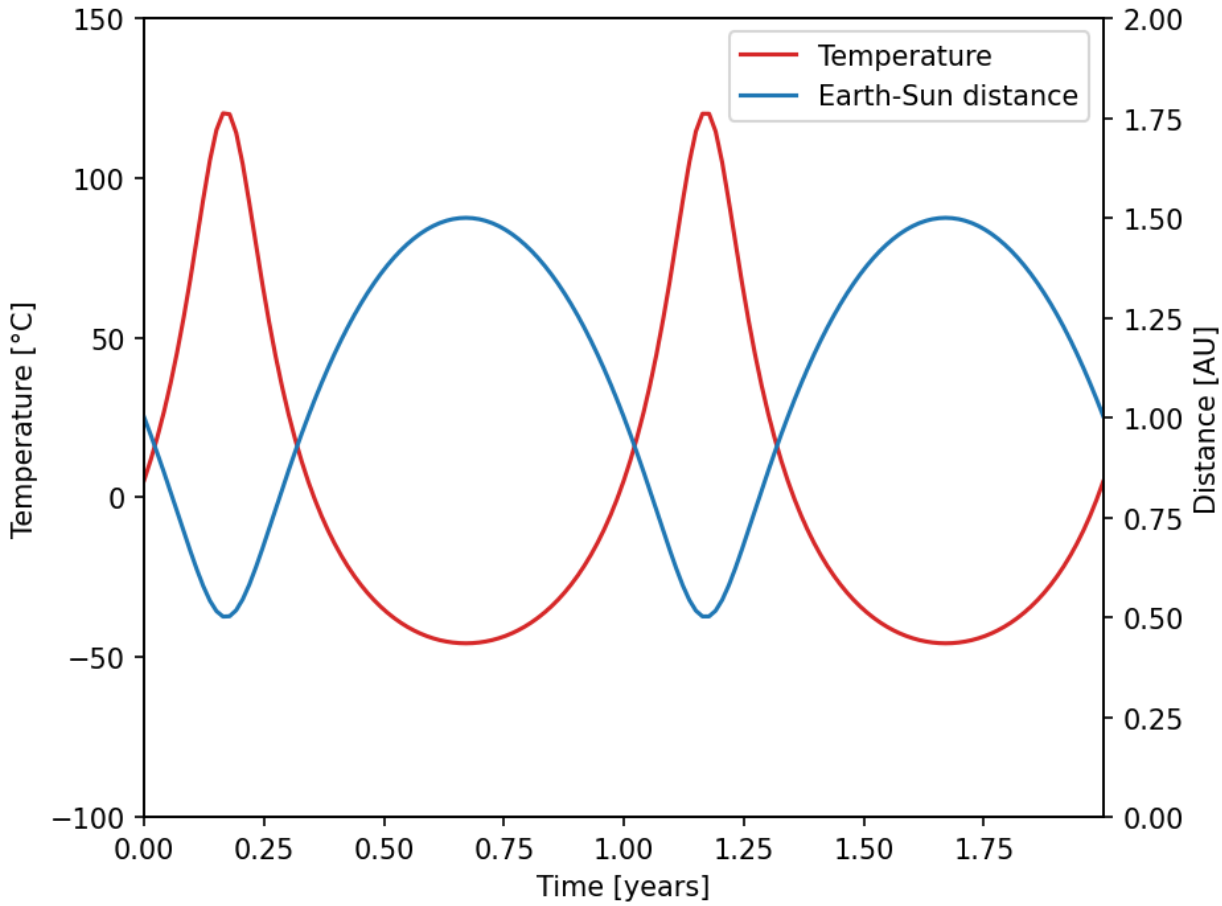
```
    fig.tight_layout()
    plt.show()
```

[58]:
```
plot_temperature(data_T)
```



3.4 The heartbeat concept

Every updater is actually performing three operations. The updater operation itself, a **"systole"**, that is executed before the update operation and a **"diastole"** that is executed after the update operation.

In this simple case we want to print Earth's temperature before and after it's calculation.

[59]:
```
def T_sys(frame):
    """This function prints the temperature before the update process."""
    msg = "{:6s}: T = {:5.1f} K".format("Before", sim.Earth.T)
    print(msg)
```

[60]:
```
def T_dia(frame):
    """This function prints the temperature after the update process."""
    msg = "{:6s}: T = {:5.1f} K".format("After", sim.Earth.T)
    print(msg)
```

We can assign these functions to systole and diastole of the temperature updater.

[61]:
```
sim.Earth.T.updater.systole = T_sys
sim.Earth.T.updater.diastole = T_dia
```

[62]:
```
sim.Earth.T = 0.
```

[63]:
```
sim.Earth.T.update()
```

```
Before: T =   0.0 K
After : T = 278.0 K
```

Note: The updater of an integration variable is not directly setting its new value. Only the integrator is setting the new value of the integration variable after all integration instructions have been executed successfully. This has the consequence, that the diastole of an integration variable *DOES NOT* have access to the updated value.

Retrieving updater information

It is possible to retrieve information about the currently assigned updater functions.

[64]:
```
sim.Earth.T.updater
```

[64]:
```
Heartbeat
---------

Systole:  <function T_sys at 0x7f951a0a4720>
Updater:  <function T at 0x7f9519454fe0>
Diastole: <function T_dia at 0x7f951a0a45e0>

Docstrings
----------

Systole:
This function prints the temperature before the update process.

Updater:
Function computes the equilibrium temperature of the Earth

Diastole:
This function prints the temperature after the update process.
```

The source code of the assigned functions can also be displayed by adressing the respective sub-level. For example the systole or the actual updater. This may not work if the assigned function is not a Python function.

[65]:
```
sim.Earth.T.updater.systole
```

[65]:
```
Updater
-------

Signature: T_sys(frame)
Source:
def T_sys(frame):
    """This function prints the temperature before the update process."""
    msg = "{:6s}: T = {:5.1f} K".format("Before", sim.Earth.T)
    print(msg)
```

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```
File: /tmp/ipykernel_24064/2382827243.py
Type: function
```

[66]:
```
sim.Earth.T.updater.updater
```

[66]:
```
Updater
-------

Signature: T(frame)
Source:
def T(frame):
    """Function computes the equilibrium temperature of the Earth"""
    return frame.Sun.T * (frame.Sun.R**2 / (4.*frame.Earth.d**2))**0.25

File: /tmp/ipykernel_24064/4057753429.py
Type: function
```

If the updater of a group was defined by assigning a list as in this example, this will be shown as well.

[67]:
```
sim.Earth.updater
```

[67]:
```
Heartbeat
---------

Systole:  None
Updater:  list_updater
Diastole: None

Docstrings
----------

Systole:
None

Updater:
The attributes in this group are updated in the order:
['d', 'T'].

Diastole:
None
```

This notebook teaches how to:
create custom integration schemes.

CHAPTER

FOUR

4. CUSTOM INTEGRATION SCHEMES

In this tutorial we want to estimate π with the following equation:

$$\pi = 4 \int_0^1 \sqrt{1-t^2} \mathrm{d}t$$

We set up the simulation frame as explained in the previous tutorials.

[1]:
```
from simframe import Frame
```

[2]:
```
sim = Frame()
```

Adding field for :math:`pi` and integration variable

[3]:
```
sim.addfield("pi", 0., description="Approximation of pi")
sim.addintegrationvariable("t", 0.)
```

Differentiator

[4]:
```
import numpy as np

def f(frame, x, Y):
    return 4.*np.sqrt(1-x**2)
```

[5]:
```
sim.pi.differentiator = f
```

Step size

We set the step size to 0.25, i.e., the integral function is only evaluated four times in the simulation.

[6]:
```
def dt(frame):
    return 0.25
```

[7]:
```
sim.t.updater = dt
```

We do not need to write outputs for this model. We only have to tell the integrator when to stop the simulation, i.e., the upper bound of the integral.

[8]:
```
sim.t.snapshots = [1.]
```

Setting the integrator

[9]:
```
from simframe import Integrator
from simframe import Instruction
from simframe import schemes
```

[10]:
```
sim.integrator = Integrator(sim.t)
```

[11]:
```
sim.integrator.instructions = [Instruction(schemes.expl_1_euler, sim.pi)]
```

Running the simulation

[12]:
```
sim.run()
```

```
Execution time: 0:00:00
```

Results

[13]:
```
from IPython.display import Markdown as md
def print_table(sim):
    return md("| |$\pi$|rel. error|\n|-|-|-|\n|real|{:10.8f}||\n|approx.|{:10.8f}|{:9.3e}
↪|".format(np.pi,sim.pi,np.abs(np.pi-sim.pi)/np.pi))
```

[14]:
```
print_table(sim)
```

[14]:

	π	rel. error
real	3.14159265	
approx.	3.49570907	1.127e-01

The relative error is about 11 %.

There are in principle two way how we can improve this estimate. One is to decrease the stepsize. You can rerun the notebook with a smaller step size and compare the results.

Another method is to use more sophisticated integration schemes. We are now going to implement the 2nd-order Midpoint Method and the 4th-order Runge-Kutta method.

4.1 Writing custom integration schemes

All we have to do is write a function that takes the current value of the integration variable **x0**, the current value of the variable to be integrated **Y0**, and the step size **dx**. The function needs to return the change **dY** of our variable **Y0** after the integration. We can access the derivative of the variable with `Y0.derivative(x, Y)`.

For the midpoint method this looks as follows.

[15]:
```
def midpoint(x0, Y0, dx, *args, **kwargs):
    x1 = x0 + 0.5*dx
    Y1 = Y0 + 0.5*dx*Y0.derivative(x0, Y0)
    return dx*Y0.derivative(x1, Y1)
```

All we have to do now is to create an integration scheme from this function. This can be done by using `AbstractScheme` provided by `simframe`.

[16]:
```
from simframe.integration import Scheme
```

[17]:
```
expl_2_midpoint = Scheme(midpoint)
```

`expl_2_midpoint` is now our new integration scheme. The naming convention is `<expl/impl>_<order>_<name><_other>`.

We can now assign a new instruction set using our new method to the integrator just as with the 1st-order Euler method.

[18]:
```
sim.integrator.instructions = [Instruction(expl_2_midpoint, sim.pi)]
```

Before we restart the simulation we have to reset to the initial conditions.

[19]:
```
sim.t = 0
sim.pi = 0
```

[20]:
```
sim.run()
```

```
Execution time: 0:00:00
```

[21]:
```
print_table(sim)
```

[21]:

	π	rel. error
real	3.14159265	
approx.	3.18392922	1.348e-02

The error is now reduced to 1.3 % only by using a higher order method.

Note: the higher order method needs more operations and is therefore slower. This does not really matter in this case, but might be important for more complex simulations.

4th-order Runge-Kutta

The scheme function for the 4th-order explicit Runge-Kutta method looks as follows.

[22]:
```
def rk4(x0, Y0, dx, *args, **kwargs):
    k1 = Y0.derivative(x0          , Y0             )
    k2 = Y0.derivative(x0 + 0.5*dx, Y0 + 0.5*dx*k1)
    k3 = Y0.derivative(x0 + 0.5*dx, Y0 + 0.5*dx*k2)
    k4 = Y0.derivative(x0 +      dx, Y0 +      dx*k3)
    return dx*(1/6*k1 + 1/3*k2 + 1/3*k3 + 1/6*k4)
```

[23]:
```
expl_4_rungekutta = Scheme(rk4)
```

[24]:
```
sim.integrator.instructions = [Instruction(rk4, sim.pi)]
```

[25]:
```
sim.t = 0
sim.pi = 0
```

[26]:
```
sim.run()
```

```
Execution time: 0:00:00
```

[27]:
```
print_table(sim)
```

[27]:

	π	rel. error
real	3.14159265	
approx.	3.12118917	6.495e-03

With this method the error is reduced down to 0.6 %.

4.2 Available integration schemes

But before you take effort into developing your own integration schemes, take a look at the schemes already provided by `simframe`:

[28]:
```
_  = "|Scheme|Description|\n"
_ += "|------|-----------|\n"
for s in schemes.__dir__():
    if s == "update": continue
    if not s.startswith("_"): _ += "|"+s+"|"+schemes.__dict__[s]().description+"|\n"
md(_)
```

[28]:

Scheme	Description
expl_1_euler	Explicit adaptive 1st-order Euler method
expl_2_fehlberg_adptv	Explicit adaptive 2nd-order Fehlberg's method
expl_2_heun	Explicit 2nd-order Heun's method
expl_2_heun_euler_adptv	Explicit adaptive 2nd-order Heun-Euler method
expl_2_midpoint	Explicit 2nd-order midpoint method
expl_2_ralston	Explicit 2nd-order Ralston's method
expl_3_bogacki_shampine_adptv	Explicit adaptive 3rd-order Bogacki-Shampine method
expl_3_gottlieb_shu_adptv	Explicit adaptive 3rd-order Gottlieb-Shu method
expl_3_heun	Explicit 3rd-order Heun's method
expl_3_kutta	Explicit 3rd-order Kutta's method
expl_3_ralston	Explicit 3rd-order Ralston's method
expl_3_ssprk	Explicit 3rd-order Strong Stability Preserving Runge-Kutta method
expl_4_38rule	Explicit 4th-order 3/8 rule method
expl_4_ralston	Explicit 4th-order Ralston's method
expl_4_runge_kutta	Explicit 4th-order classical Runge-Kutta method
expl_5_cash_karp_adptv	Explicit adaptive 5th-order Cash-Karp method
expl_5_dormand_prince_adptv	Explicit adaptive 5th-order Dormand-Prince method
impl_1_euler_direct	Implicit 1st-order direct Euler method
impl_1_euler_gmres	Implicit 1st-order Euler method with GMRES solver
impl_2_midpoint_direct	Implicit 2nd-order direct midpoint method

This notebook teaches how to:

set up adaptive integration schemes, set up fail operations, set up preparation and finalization instructions, and use suggested step sizes.

CHAPTER

FIVE

5. ADAPTIVE INTEGRATION SCHEMES

For this tutorial we revisit the problem of the first tutorial.

- $\frac{\mathrm{d}Y}{\mathrm{d}x} = b\,Y$
- $Y\,(0) = A$
- $Y\,(x) = A\,e^{bx}$

But this time we increase the step size, such that the numeric solution is oscillating.

Problem parameters

[1]:
```
dx =  1.75
A  =  1.
b  = -1.
```

Setting up frame

[2]:
```
from simframe import Frame

sim = Frame(description="Adaptive step sizing")
```

Adding field and integration variable

[3]:
```
sim.addintegrationvariable("x", 0.)
sim.addfield("Y", A)
```

Setting up writer

[4]:
```
from simframe import writers
```

[5]:
```
sim.writer = writers.namespacewriter()
sim.writer.verbosity = 0
```

Setting differential equation

We slightly modify the differential equation and add a counter that tells us how often the function got called.

[6]:
```
N = 0
```

[7]:
```
def dYdx(frame, x, Y):
    global N
    N += 1
    return b*Y
```

[8]:
```
sim.Y.differentiator = dYdx
```

Setting up the step size

In this example we return a constant step size defined previously.

[9]:
```
def fdx(frame):
    return dx
```

[10]:
```
sim.x.updater = fdx
```

Setting up snapshots

[11]:
```
import numpy as np
sim.x.snapshots = np.arange(dx, 15., dx)
```

Setting up integrator

First we simply integrate with the known 1st-order Euler scheme with a constant step size.

[12]:
```
from simframe import Integrator
from simframe import Instruction
from simframe import schemes
```

[13]:
```
sim.integrator = Integrator(sim.x)
```

[14]:
```
sim.integrator.instructions = [Instruction(schemes.expl_1_euler, sim.Y)]
```

Running the simulation

[15]:
```
sim.run()
```

```
Execution time: 0:00:00
```

Reading data

[16]:
```
data = sim.writer.read.all()
```

We store the data in a list for later comparison.

[17]:
```
dataset = []
dataset.append([data, "Euler 1st-order", N])
```

Plotting

Function returning the exact solution used for plotting

[18]:
```
def f(x):
    return A*np.exp(b*x)
```

[19]:
```
import matplotlib.pyplot as plt

def plot(dataset):
    fig, ax = plt.subplots(dpi=150)
    x = np.linspace(0, 15., 100)
```

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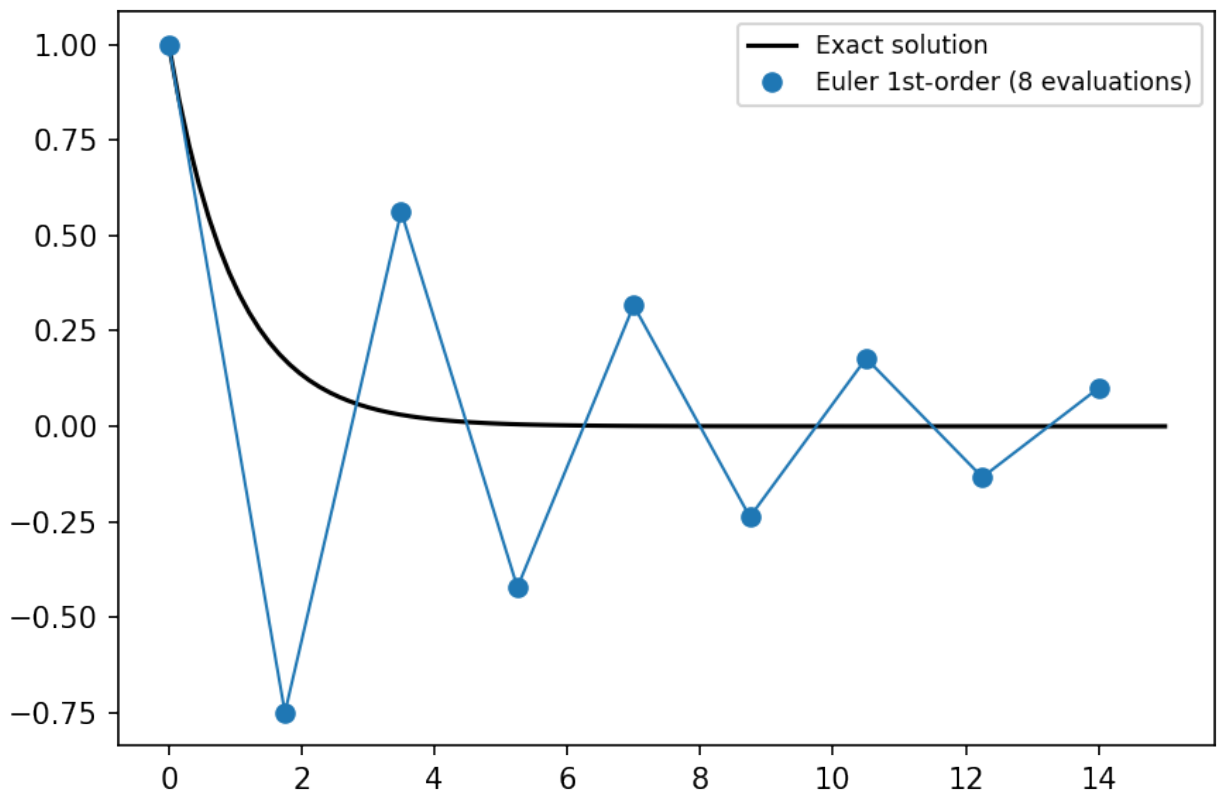
```
    ax.plot(x, f(x), c="black", label="Exact solution")
    for i, val in enumerate(dataset):
        ax.plot(val[0].x, val[0].Y, "o", c="C"+str(i), label="{} ({} evaluations)".
↪format(val[1], val[2]))
        ax.plot(val[0].x, val[0].Y, c="C"+str(i), lw=1)
    ax.legend(fontsize="small")
    fig.tight_layout()
    plt.show()
```

[20]:
```
plot(dataset)
```



As you can see, the calculated solution is oscillating aroung the real solution.

5.1 Adaptive Step Sizing Schemes

Instead of a constant step size, we now want to adjust it dynamically. If the error is too large, we decrease the step size. As an estimate for the error we compare the full Euler 1st-order step to the solution we get from performing two consecutive Euler 1st-order step with half the step size. If the relative error is larger than 10 %, we repeat the integration with a smaller step size until we are withing the error.

We therefore have to set up a custom integration scheme as was shown in the previous example. The scheme has to perform the full step and two semi steps and and needs to compare them. If the error is too large, the scheme has to return `False`. If it was successful, it has to return the change `dY` of the dependent variable `Y`.

[21]:
```
def adaptive(x0, Y0, dx, *args, **kwargs):
    fullstep  = dx*Y0.derivative(x0, Y0)
    semistep1 = 0.5*fullstep
    semistep2 = 0.5*dx*Y0.derivative(x0+0.5*dx, Y0+semistep1)
    semisteps = semistep1 + semistep2

    relerr = np.abs((semisteps-fullstep)/(Y0+semisteps))

    if relerr > 0.1:
        return False
    else:
        return semisteps
```

Creating scheme and modifying instruction set

[22]:
```
from simframe.integration import Scheme
adaptive = Scheme(adaptive)
sim.integrator.instructions = [Instruction(adaptive, sim.Y)]
```

5.2 The fail operation

If the integration failed, because the step size was too large, i.e., the scheme returned `False`, the integrator triggers a fail operation. This operation can be used to manipulate the step size. In our case, we want to decrease the step size by a factor of 10.

Note the `global dx` to manipule `dx` persistently outside the function.

[23]:
```
def failop(frame):
    global dx
    dx /= 10.
```

We assign this function to the fail operation of the integrator. The fail operation needs the parent `Frame` object as positional argument. If any instruction returns `False`, the fail operation will be executed and the integrator goes through the instructions again, before updating the fields.

Note: In case you have an `update` instuction in your instruction set, you have to undo it by yourself in the fail operation.

[24]:
```
sim.integrator.failop = failop
```

5.3 Preparation and finalization

If the integration was successful, we want to increase our step size by a factor of 5. This is done via the `finalizer` of the integrator, which is called after going through the instruction set and after updating the fields to be integrated. The equivalent that is called before going through the instructions set is `<Frame>.integrator.preparator`.

[25]:
```
def finalize(frame):
    global dx
    dx *= 5.
```

[26]:
```
sim.integrator.finalizer = finalize
```

Resetting the parameters

[27]:
```
N = 0
sim.x = 0.
sim.Y = 1.
sim.writer.reset()
```

Before running the simulation we save the inital step size for later use.

[28]:
```
import copy
dx_ini = dx
```

Running the simulation

[29]:
```
sim.run()
```

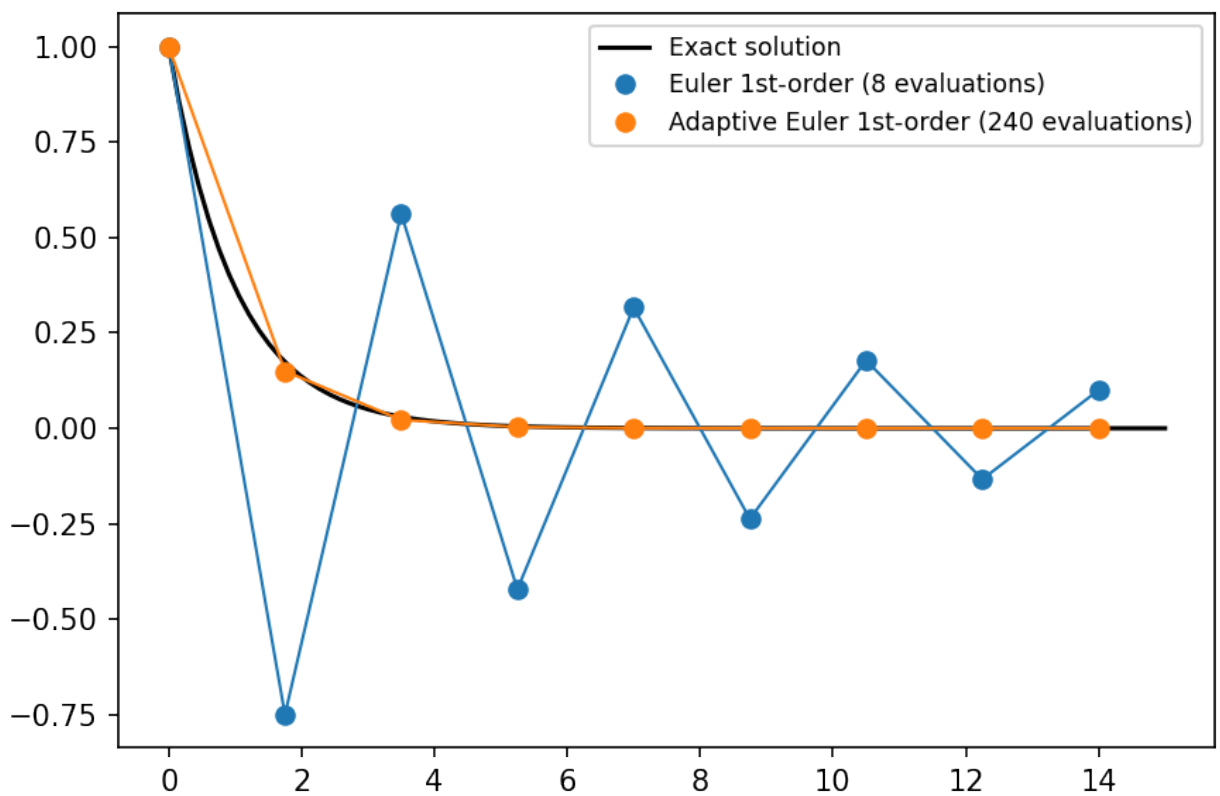
```
Execution time: 0:00:00
```

Reading data and plotting

[30]:
```
data_adaptive = sim.writer.read.all()
```

[31]:
```
dataset.append([data_adaptive, "Adaptive Euler 1st-order", N])
```

[32]:
```
plot(dataset)
```



Embedded methods

Another technique for estimating the error is to perform a higher order method for the full step instead of the same method for two semistep as done before. In some cases the higher order method is utilizing the result of the lower order method, saving evaluations. These methods are called embedded methods.

`simframe` comes with a few embedded methods. In this example we use the embedded Bogacki-Shampine method.

[33]:
```
sim.integrator.instructions = [Instruction(schemes.expl_3_bogacki_shampine_adptv, sim.Y)]
```

5.4 Suggested step sizes

The embedded methods included in `simframe` provide an estimate for the new step size depending on the truncation error. This estimate is saved in the integration variable in `<IntVar>.suggested`. We have to modify the step size function to utilize this estimate.

[34]:
```
def fdx(sim):
    return sim.x.suggested
```

[35]:
```
sim.x.updater = fdx
```

And we have to give an initial suggestion for the step size. We'll use the initial value as before.

[36]:
```
sim.x.suggest(dx_ini)
```

Unsetting fail operation and finalization

The fail operation and finalization operations are not needed anymore and have to be unset.

[37]:
```
sim.integrator.failop = None
sim.integrator.finalizer = None
```

Resetting the parameters and running the simulation

[38]:
```
N = 0
sim.x = 0.
sim.Y = 1.
sim.writer.reset()
```

[39]:
```
sim.run()
```

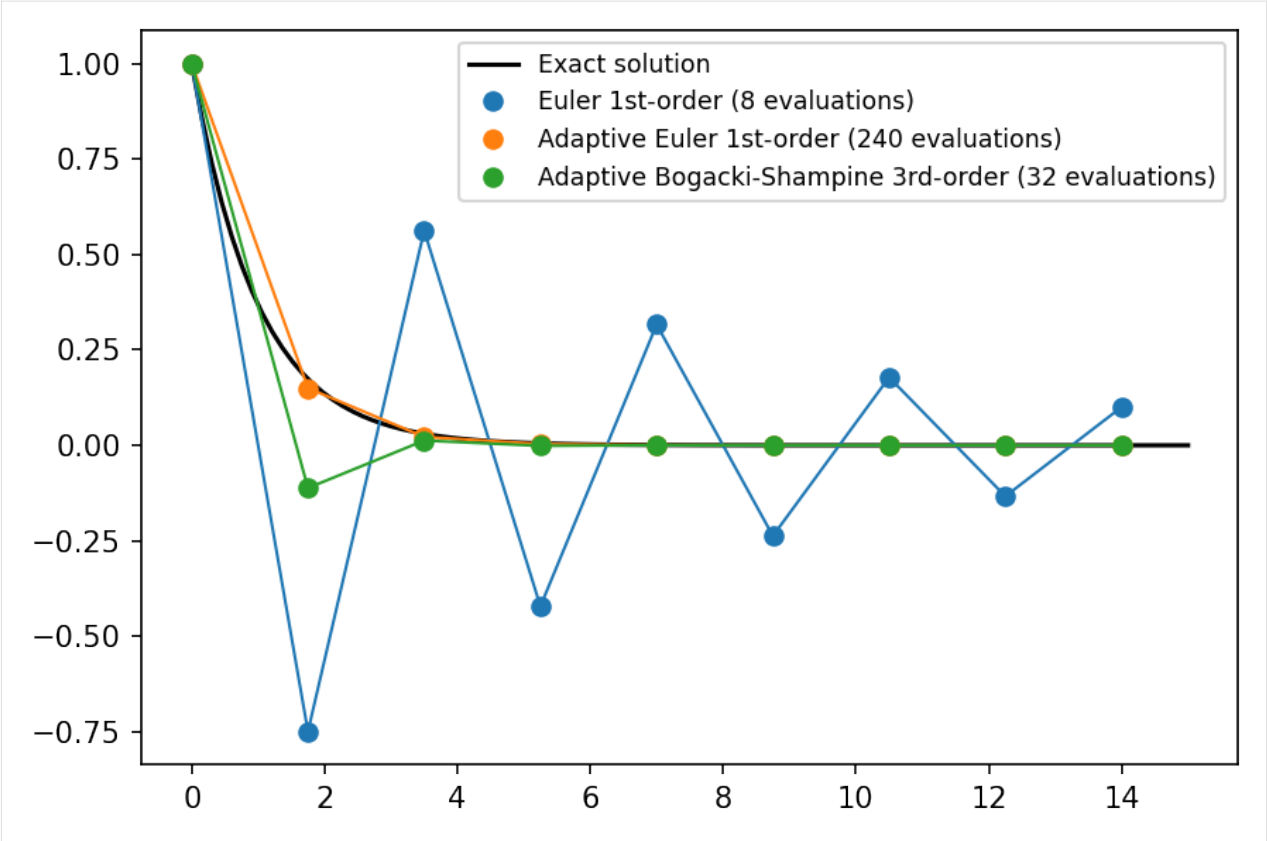
```
Execution time: 0:00:00
```

Reading data and plotting

[40]:
```
data_bogackishampine = sim.writer.read.all()
```

[41]:
```
dataset.append([data_bogackishampine, "Adaptive Bogacki-Shampine 3rd-order", N])
```

[42]:
```
plot(dataset)
```



As you can see the Bogacki-Shampine method needs 32 eveluations of the derivative in this setup. That's only about half of the amount of the adaptive Euler method and it's significantly more accurate.

Change the stepsize to `dx = 2.25` and run the notebook again. For this step size the Euler 1st-order method is unstable.

5.5 Passing keyword arguments to integration scheme

It is also possible to pass key word arguments to the integrator to control its behaviour. We could for example increase the accuracy by changing the desired relative error. This is done by passing a controller dictionary to the instruction.

[43]:
```
sim.integrator.instructions = [Instruction(schemes.expl_3_bogacki_shampine_adptv, sim.Y,␣
↪controller={"eps": 0.01})]
```

Here we want to have maximum relative error of $1\,\%$. Default is $10\,\%$.

Resetting the parameters and running the simulation

Note the `reset=True` keyword when resetting the suggested step size. Suggesting step sizes takes the minimum of the suggested and the current value, which is still set from the earlier integration. We therefore have to reset the current value with the keyword.

[44]:
```
N = 0
sim.x = 0.
sim.x.suggest(dx_ini, reset=True)
sim.Y = 1.
```

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```
sim.Y._buffer = None
sim.writer.reset()
```

[45]:
```
sim.run()
```

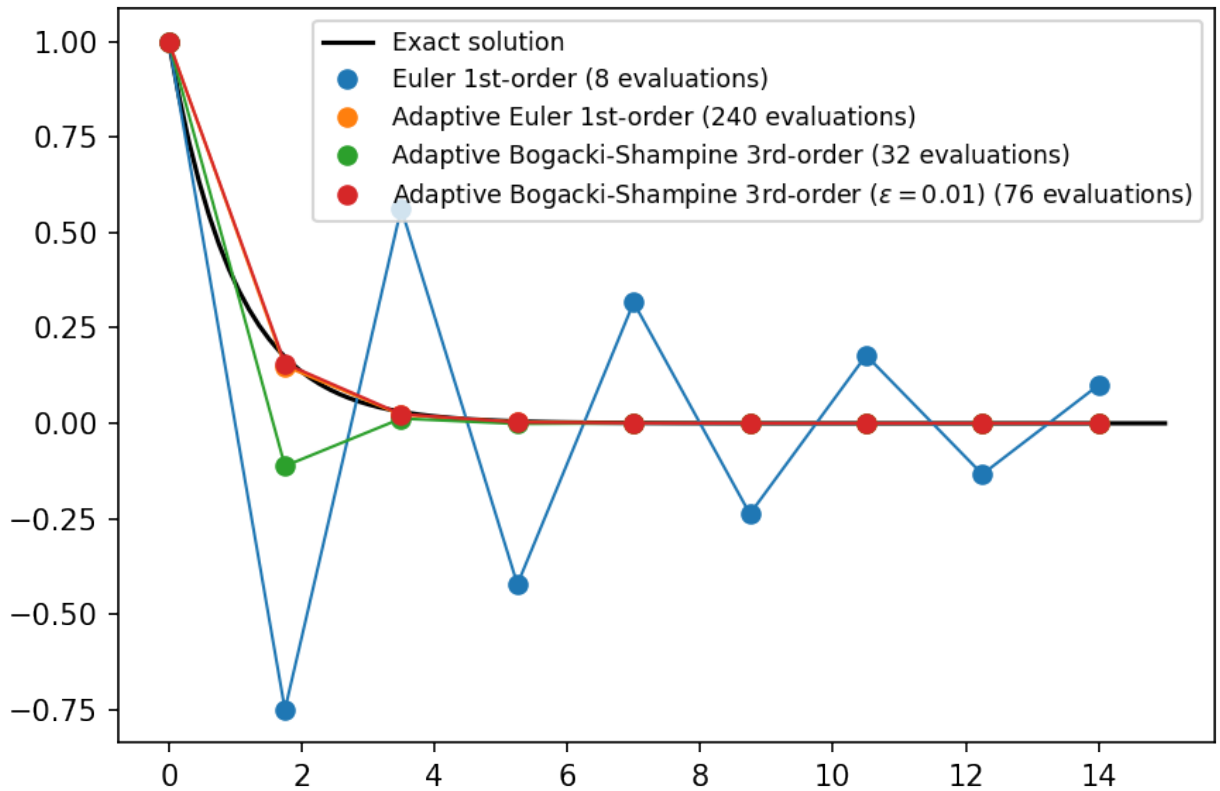
```
Execution time: 0:00:00
```

Reading and plotting data

[46]:
```
data_bogackishampine_accurate = sim.writer.read.all()
```

[47]:
```
dataset.append([data_bogackishampine_accurate, "Adaptive Bogacki-Shampine 3rd-order ($\
↪epsilon=0.01$)", N])
```

[48]:
```
plot(dataset)
```



With this settings it takes slightly longer to approach the analytical solution, but the overshooting in the beginning is prevented.

This notebook teaches how to:

set up implicit integration schemes.

CHAPTER

SIX

6. IMPLICIT INTEGRATION

In this example we revisit the differential equation from the first tutorial and the last tutorial about adaptive scheme.

For this tutorial we revisit the problem of the first tutorial.

- $\frac{\mathrm{d}Y}{\mathrm{d}x} = b\,Y$
- $Y\left(0\right) = A$
- $Y\left(x\right) = A\,e^{bx}$

But this time we increase the step size, such that the 1st-order Euler scheme is unstable.

Analytic solution

[1]:
```
import numpy as np
```

[2]:
```
def f(x, A, b):
    return np.exp(b*x)
```

Model parameters

[3]:
```
A  =   1.
b  =  -1.
dx =  10.
```

This time we chose a large step size and set up the frame.

[4]:
```
from simframe import Frame
```

[5]:
```
sim_expl = Frame(description="Explicit integratioon")
```

[6]:
```
sim_expl.addfield("Y", A)
sim_expl.addintegrationvariable("x", 0.)
```

[7]:
```
def fdx(frame):
    return dx
sim_expl.x.updater = fdx
sim_expl.x.snapshots = [10.]
```

[8]:
```
def diff_expl(frame, x, Y):
    return b*Y
sim_expl.Y.differentiator = diff_expl
```

[9]:
```
from simframe import Integrator
from simframe import Instruction
from simframe import schemes
```

[10]:
```
sim_expl.integrator = Integrator(sim_expl.x)
sim_expl.integrator.instructions = [Instruction(schemes.expl_1_euler, sim_expl.Y)]
```

[11]:
```
from simframe import writers
```

[12]:
```
sim_expl.writer = writers.namespacewriter()
sim_expl.writer.verbosity = 0
```

[13]:
```
sim_expl.run()
```

```
Execution time: 0:00:00
```

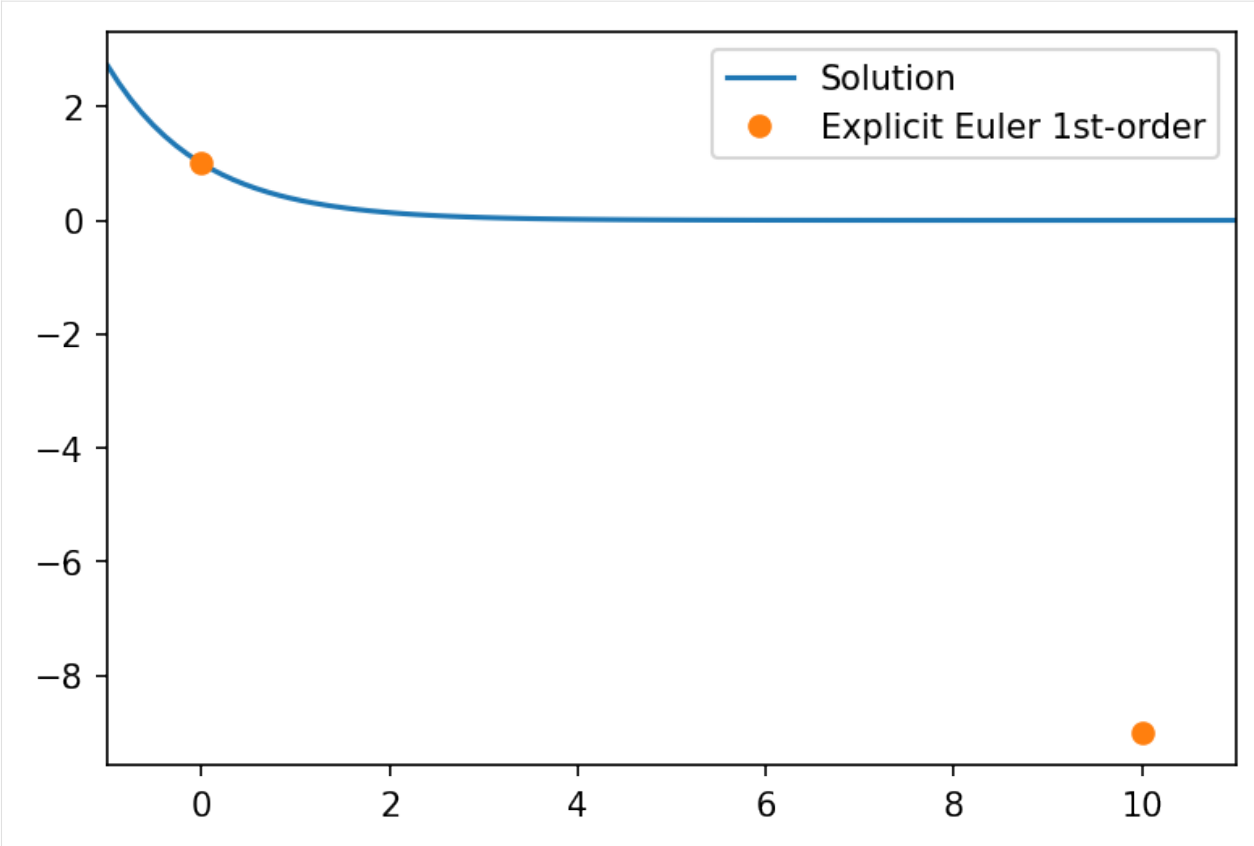
Reading data and plotting

[14]:
```
data_expl = sim_expl.writer.read.all()
```

[15]:
```
import matplotlib.pyplot as plt

def plot(ls):
    fig, ax = plt.subplots(dpi=150)
    x = np.linspace(-1., 11, 100)
    ax.set_xlim(x[0], x[-1])
    ax.plot(x, f(x, A, b), label="Solution")
    for sim, d in ls:
        ax.plot(sim.x, sim.Y, "o", label=d)
    ax.legend()
    plt.show()
```

[16]:
```
plot([(data_expl, "Explicit Euler 1st-order")])
```



In this case the step width is way too large to produce a useful result.

The only help would be to reduce the step size or to go for implicit integration.

6.1 Background: Implicit integration

For explicit integration the derivative f of the differential equation is evaluated at the current point in time or space:

$\frac{\Delta Y}{\Delta x} = \frac{Y_{n+1} - Y_n}{\Delta x} = f\left(Y_n\right),$

which leads to the simple 1st-order Euler scheme.

$Y_{n+1} = Y_n + \Delta x \, f\left(Y_n\right).$

Implicit integration means that the derivative is evaluated at the future point in time or space:

$\frac{Y_{n+1} - Y_n}{\Delta x} = f\left(Y_{n+1}\right).$

What looks ridiculous at first is mathematically sound.

Imagine that the derivative can be written as a matrix equation.

$f\left(\vec{Y}\right) = \mathbf{J} \cdot \vec{Y},$

with the Jacobian matrix $\mathbf{J}$.

Plugging this into our differential equation yields

$\vec{Y}_{n+1} - \vec{Y}_n = \Delta x \, \mathbf{J} \cdot \vec{Y}_{n+1}$

$\Leftrightarrow (\mathbb{1} - \Delta x\, \mathbb{J}) \cdot \vec{Y}_{n+1} = \vec{Y}_n$

$\Leftrightarrow \vec{Y}_{n+1} = (\mathbb{1} - \Delta x\, \mathbb{J})^{-1} \cdot \vec{Y}_n$

The solution can be found by inverting the matrix $\mathbb{1} - \Delta x\, \mathbb{J}$.

In our simple case this translates to

$\mathbb{J} = (b)$

and

$Y_{n+1} = \frac{1}{1-\Delta x\, b} Y_n$

For large step sizes $(\Delta\, x \to \infty)$ this goes to zero $(Y_n \to 0)$ as it should compared to the exact solution. The integration scheme is *"unconditionally stable"*.

6.2 Setting up implicit integration

Setting up implicit integration is similar to explicit integration. We therefore just copy our frame and reset the values.

[17]:
```
import copy
```

[18]:
```
sim_impl = copy.deepcopy(sim_expl)
sim_impl.x = 0
sim_impl.Y = A
sim_impl.writer.reset()
```

The important difference is now, that instead of the derivative we have to provide the Jacobian $\mathbb{J}$ to our field Y, which is in our case very simple. The function for the Jacobi matrix needs the parent frame object as first and the integration variable as second positional argument.

[19]:
```
def jac_impl(sim, x):
    return np.array([b])
sim_impl.Y.jacobinator = jac_impl
```

We can now use an implicit scheme in our instruction set.

[20]:
```
sim_impl.integrator.instructions = [Instruction(schemes.impl_1_euler_direct, sim_impl.Y)]
```

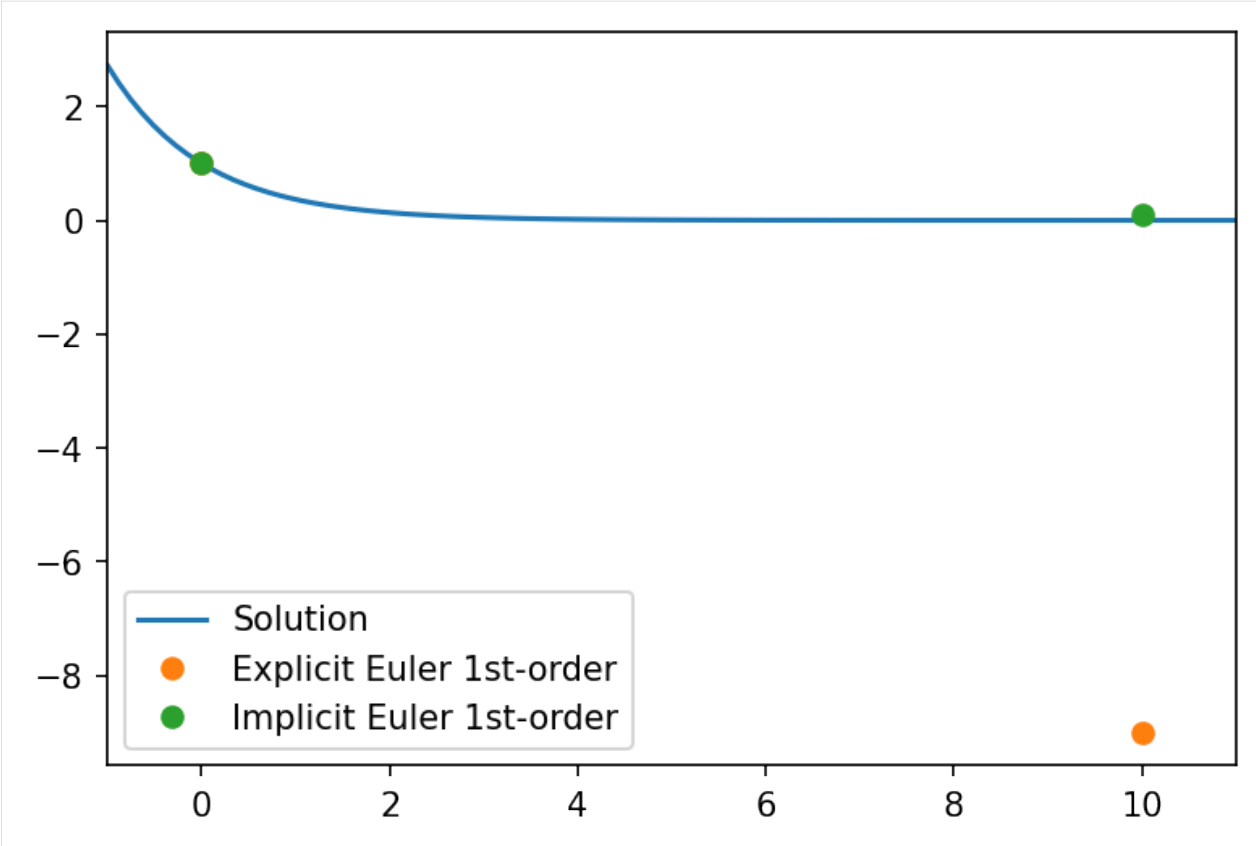
Now we can rerun the simulation.

[21]:
```
sim_impl.run()
```

```
Execution time: 0:00:00
```

[22]:
```
data_impl = sim_impl.writer.read.all()
```

[23]:
```
plot([(data_expl, "Explicit Euler 1st-order"),(data_impl, "Implicit Euler 1st-order")])
```



Since implicit schemes involve matrix inversions, it can be very costly. The method shown here uses `numpy.linalg.inv()` to compute the inverse matrix, which is basically Gaussian elimination with LU factorization. There are other methods that might be more suitable for your problem.

Note: If the jacobinator is set, but not the differentiator, `simframe` will try to calculated the derivative from the Jacobi matrix by assuming

$\vec{Y}' = \mathbb{J} \cdot \vec{Y}$

[24]:
```
sim_impl.Y.differentiator = None     # unsetting the differentiator
```

[25]:
```
sim_impl.Y.derivative()
```

[25]:
```
-0.09090909090909094
```

Only if neither the differentiator, nor the jacobinator are set, `Field.derivative()` will return zeros in the shape of the field, i.e., the derivative is zero.

[26]:
```
sim_impl.Y.jacobinator = None
```

[27]:
```
sim_impl.Y.derivative()
```

[27]:
```
0.0
```

CHAPTER

SEVEN

EXAMPLE: COUPLED OSCILLATORS

In this example we'll have a look at coupled oscillations of two bodies with masses m_i connected via three springs to themselves and attached to walls. The goal is to calculate the time evolution of this system if it's not in equilibrium. The springs have spring constants of k_i and lengths of l_i when no forces are acting on them. The distance between the walls is L.

[1]:
```
k1, l1 = 10., 6.
k2, l2 = 20., 6.
k3, l3 = 10., 6.

m1, m2 = 1., 1.

L = 15.
```

Springs connected serially have a resulting spring constant of K, which is the inverse sum of the individual spring constants.

[2]:
```
Kinv = 1./k1 + 1./k2 + 1./k3
K    = 1./Kinv
```

The force exerted by a spring is given by

$\vec{F} = -k \cdot \vec{d}$

where $\vec{d}$ is the displacement vector from its equilibrium position. The system can be more easily solved by solving for the time evolution of the displacements $\vec{d_i}$ of the bodies. To convert it back into actual coordinates, we first have to finde the equilibrium positions $\vec{x}_i$ of the bodies.

If the system is in equilibrium, the forces acting on each individual spring are identical.

[3]:
```
F = - ( L - ( l1 + l2 + l3 ) ) * K
```

From this we can calculate the equilibrium positions.

[4]:
```
x1 = l1 - F/k1
```

[5]:
```
x2 = F/k3 + L - l3
```

In equilibrium our system looks as follows.

[6]:
```
import matplotlib.pyplot as plt
import matplotlib.patches as patches
import numpy as np
```

[7]:
```
def getspring(l1, l2, bw):
    l1 = float(l1)
    l2 = float(l2)
    bw = float(bw)
    L = l2 - l1
    d = L/6.
    x = np.array([l1, d, d/2., d, d, d, d/2., d], dtype=float)
    for i in range(1, 8):
        x[i] += x[i-1]
    y = np.array([0., 0., 2.*bw, -2.*bw, 2.*bw, -2*bw, 0., 0.], dtype=float)
    return x, y
```

[8]:
```
def plot_system(bw, x1, x2, L):

    fig, ax = plt.subplots(dpi=150)
    ax.axis("off")
    ax.set_aspect(1.)

    rectl = patches.Rectangle((-bw, -4.*bw), bw, 8.*bw, linewidth=1, edgecolor="#000000",
↪ facecolor="#dddddd", hatch="//")
    ax.add_patch(rectl)
    rectr = patches.Rectangle((L, -4.*bw), bw, 8.*bw, linewidth=1, edgecolor="#000000",␣
↪facecolor="#dddddd", hatch="//")
    ax.add_patch(rectr)
    body1 = patches.Circle((x1, 0), bw, linewidth=1, edgecolor="#000000", facecolor="C1")
    ax.add_patch(body1)
    body2 = patches.Circle((x2, 0), bw, linewidth=1, edgecolor="#000000", facecolor="C9")
    ax.add_patch(body2)

    s1x, s1y = getspring(0., x1-bw, bw)
    ax.plot(s1x, s1y, c="#000000", lw=1)

    s2x, s2y = getspring(x1+bw, x2-bw, bw)
    ax.plot(s2x, s2y, c="#000000", lw=1)

    s3x, s3y = getspring(x2+bw, L, bw)
    ax.plot(s3x, s3y, c="#000000", lw=1)

    ax.set_xlim(-2.*bw, L+2.*bw)
    ax.set_ylim(-3., 3.)

    fig.tight_layout()

    return fig, ax
```

[9]:
```
bw = 0.5
fig, ax = plot_system(bw, x1, x2, L)

ax.text((x1+0.)/2., 3*bw, "$k_1$", verticalalignment="center", horizontalalignment=
↪"center")
ax.text((x2+x1)/2., 3*bw, "$k_2$", verticalalignment="center", horizontalalignment=
↪"center")
```

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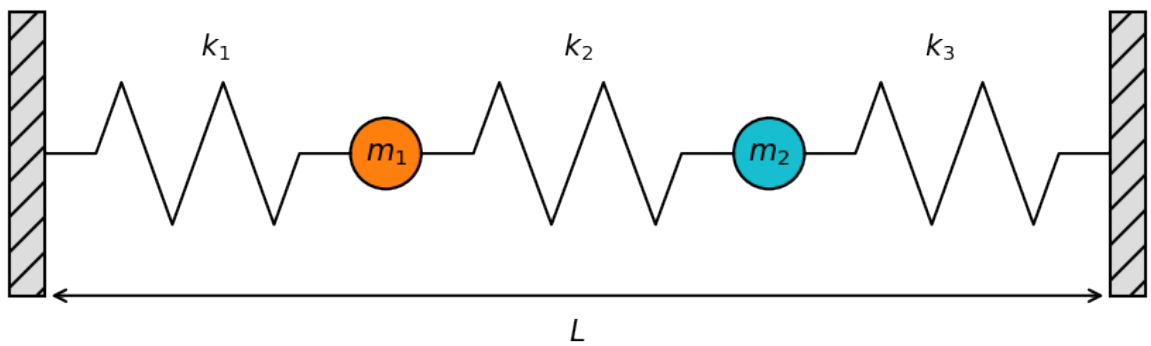
```
ax.text((L +x2)/2., 3*bw, "$k_3$", verticalalignment="center", horizontalalignment=
↪"center")

ax.text(x1, 0., "$m_1$", verticalalignment="center", horizontalalignment="center")
ax.text(x2, 0., "$m_2$", verticalalignment="center", horizontalalignment="center")

ax.annotate(text='', xy=(0., -4.*bw), xytext=(L, -4.*bw), arrowprops=dict(arrowstyle='<->
↪', lw=1))
ax.text(L/2, -5.*bw, "$L$", verticalalignment="center", horizontalalignment="center")

plt.show()
```



We know want to displace mass m_1 from its equilibrium position and calculate the time evolution of the whole system.

The force acting on m_1 is given by

$F_1 = m\dot{v_1} = -(k_1 + k_2) \cdot d_1 + k_2 \cdot d_2$

Vector notation is ommited since the problem is one-dimensional. The change in the displacement d_1 is given by

$\dot{d_1} = v_1$

Similarily for the second body

$F_2 = m\dot{v_2} = -(k_2 + k_3) \cdot d_2 + k_2 \cdot d_1$

$\dot{d_2} = v_2$

This is a system of coupled differential equations that can be written in matrix form

$$\begin{pmatrix} \dot{d_1} \\ \dot{d_2} \\ \dot{v_1} \\ \dot{v_2} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -\frac{k_1+k_2}{m_1} & \frac{k_2}{m_1} & 0 & 0 \\ \frac{k_2}{m_2} & -\frac{k_2+k_3}{m_2} & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} d_1 \\ d_2 \\ v_1 \\ v_2 \end{pmatrix}$$

or short

$\frac{\mathrm{d}}{\mathrm{d}t}\vec{Y} = \mathbf{J} \cdot \vec{Y}$

with the state vector $\vec{Y}$ and the Jacobian $\mathbf{J}$.

We can now start setting up the frame.

[10]:
```
from simframe import Frame
```

[11]:
```
sim = Frame(description="Coupled Oscillators")
```

[12]:
```
import numpy as np
```

[13]:
```
Y = np.array([-3., 0., 0., 0.])
sim.addfield("Y", Y, description="State vector")
```

In this configuration mass m_1 is displaced by 3 to the left while m_2 is in its equilibrium position. Both bodies are at rest.

We set up the time as integration variable.

[14]:
```
sim.addintegrationvariable("t", 0., description="Time")
```

[15]:
```
def dt(sim):
    return 0.1
```

[16]:
```
sim.t.updater = dt
```

We define the snapshots according the frames per second and maximum simulation time that we want to have in the animation later.

[17]:
```
fps = 30.
t_max = 15.
```

[18]:
```
sim.t.snapshots = np.arange(1./fps, t_max, 1./fps)
```

In principle this would be enough to run the simulation. But for convenience we set up a few more fields and groups.

[19]:
```
sim.addgroup("b1", description="Body 1")
sim.addgroup("b2", description="Body 2")

# Body 1
sim.b1.addfield("m" , m1, description="Mass", constant=True)
sim.b1.addfield("d" , 0., description="Displacement")
sim.b1.addfield("x" , 0., description="Position")
sim.b1.addfield("x0", x1, description="Equilibrium Position", constant=True)
sim.b1.addfield("v" , 0., description="Velocity")

# Body 2
sim.b2.addfield("m" , m2, description="Mass", constant=True)
sim.b2.addfield("d" , 0., description="Displacement")
sim.b2.addfield("x" , 0., description="Position")
sim.b2.addfield("x0", x2, description="Equilibrium Position", constant=True)
sim.b2.addfield("v" , 0., description="Velocity")
```

These fields need to be updated from the state vector.

[20]:
```
# Body 1
def update_d1(sim):
```

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```
    return sim.Y[0]
sim.b1.d.updater = update_d1
def update_v1(sim):
    return  sim.Y[2]
sim.b1.v.updater = update_v1
def update_x1(sim):
    return sim.b1.x0 + sim.b1.d
sim.b1.x.updater = update_x1

# Body 2
def update_d2(sim):
    return sim.Y[1]
sim.b2.d.updater = update_d2
def update_v2(sim):
    return  sim.Y[3]
sim.b2.v.updater = update_v2
def update_x2(sim):
    return sim.b2.x0 + sim.b2.d
sim.b2.x.updater = update_x2
```

And we are adding more groups for the spring parameters.

[21]:
```
sim.addgroup("s1", description="Spring 1")
sim.addgroup("s2", description="Spring 2")
sim.addgroup("s3", description="Spring 3")

sim.s1.addfield("k", k1, description="Spring Constant", constant=True)
sim.s1.addfield("l", l1, description="Length", constant=True)
sim.s2.addfield("k", k2, description="Spring Constant", constant=True)
sim.s2.addfield("l", l2, description="Length", constant=True)
sim.s3.addfield("k", k3, description="Spring Constant", constant=True)
sim.s3.addfield("l", l3, description="Length", constant=True)
```

We now have to tell `simframe` in what order to update the fields.

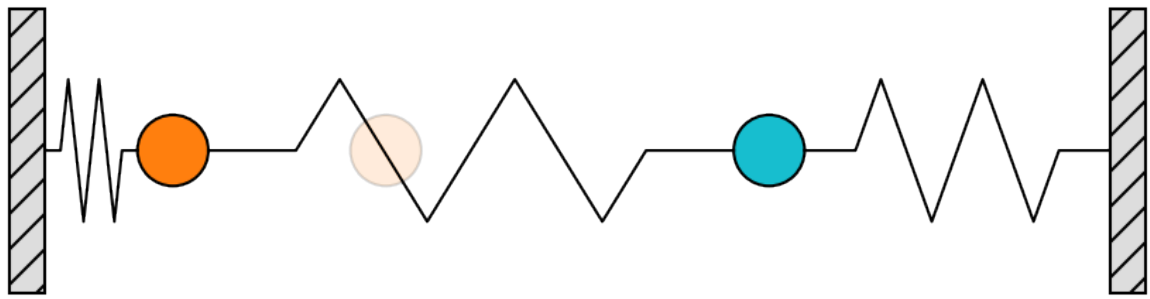
[22]:
```
# The groups for the bodies. The order does not matter
sim.updater = ["b1", "b2"]
# The fields in the groups. Displacement has to be updated before position
sim.b1.updater = ["d", "v", "x"]
sim.b2.updater = ["d", "v", "x"]
```

We can now fill the fields with their initial conditions from the state vector.

[23]:
```
sim.update()
```

The initial state of the system looks as follows:

[24]:
```
fig, ax = plot_system(0.5, sim.b1.x, sim.b2.x, L)
circ = patches.Circle((sim.b1.x0, 0.), 0.5, linewidth=1, edgecolor="#000000", facecolor=
↪"C1", alpha=0.15)
ax.add_patch(circ)
plt.show()
```



Printing the complete frame structure

[25]:
```
sim.toc
```

```
Frame (Coupled Oscillators)
    - b1: Group (Body 1)
        - d: Field (Displacement)
        - m: Field (Mass), constant
        - v: Field (Velocity)
        - x: Field (Position)
        - x0: Field (Equilibrium Position), constant
    - b2: Group (Body 2)
        - d: Field (Displacement)
        - m: Field (Mass), constant
        - v: Field (Velocity)
        - x: Field (Position)
        - x0: Field (Equilibrium Position), constant
    - s1: Group (Spring 1)
        - k: Field (Spring Constant), constant
        - l: Field (Length), constant
    - s2: Group (Spring 2)
        - k: Field (Spring Constant), constant
        - l: Field (Length), constant
    - s3: Group (Spring 3)
        - k: Field (Spring Constant), constant
        - l: Field (Length), constant
    - t: IntVar (Time), Integration variable
    - Y: Field (State vector)
```

Setting up the Jacobian

For implicit schemes we have to calculate the Jacobian. Since in this case the Jacobian is constant with time, we can define it outside of the frame object.

[26]:
```
jac = np.array([[          0.,           0., 1., 0.],
                [          0.,           0., 0., 1.],
                [-(k1+k2)/m1,        k2/m1, 0., 0.],
                [       k2/m2, -(k2+k3)/m2, 0., 0.]], dtype=float)
```

[27]:
```
jac
```

[27]:
```
array([[  0.,   0.,   1.,   0.],
       [  0.,   0.,   0.,   1.],
       [-30.,  20.,   0.,   0.],
       [ 20., -30.,   0.,   0.]])
```

[28]:
```
def jac_impl(sim, x):
    return jac
```

[29]:
```
sim.Y.jacobinator = jac_impl
```

Setting up the Integrator

We can now set up the integrator just as in the previous examples.

[30]:
```
from simframe import Integrator
from simframe import Instruction
from simframe import schemes
```

[31]:
```
sim.integrator = Integrator(sim.t)
```

[32]:
```
sim.integrator.instructions = [Instruction(schemes.impl_1_euler_direct, sim.Y)]
```

Setting up the Writer

We also have to set up the writer. In this case we don't want to write data files. So we simply write the data into a namespace

[33]:
```
from simframe import writers
```

[34]:
```
sim.writer = writers.namespacewriter()
sim.writer.verbosity = 0
```

Starting the simulation

[35]:
```
sim.run()
```

```
Execution time: 0:00:01
```

Reading data

[36]:
```
data = sim.writer.read.all()
```

[37]:
```
def plot_oszillations(data):
    fig, ax = plt.subplots(dpi=150)
    ax.plot(data.b1.x, data.t, c="C1")
    ax.plot(data.b2.x, data.t, c="C9")
    ax.axvline(data.b1.x0[0], c="#000000", alpha=0.5, lw=1)
    ax.axvline(data.b2.x0[0], c="#000000", alpha=0.5, lw=1)
    ax.set_xlim(0, L)
    ax.set_ylim(data.t[-1], data.t[0])
    ax.set_xlabel("Position")
    ax.set_ylabel("Time")
```

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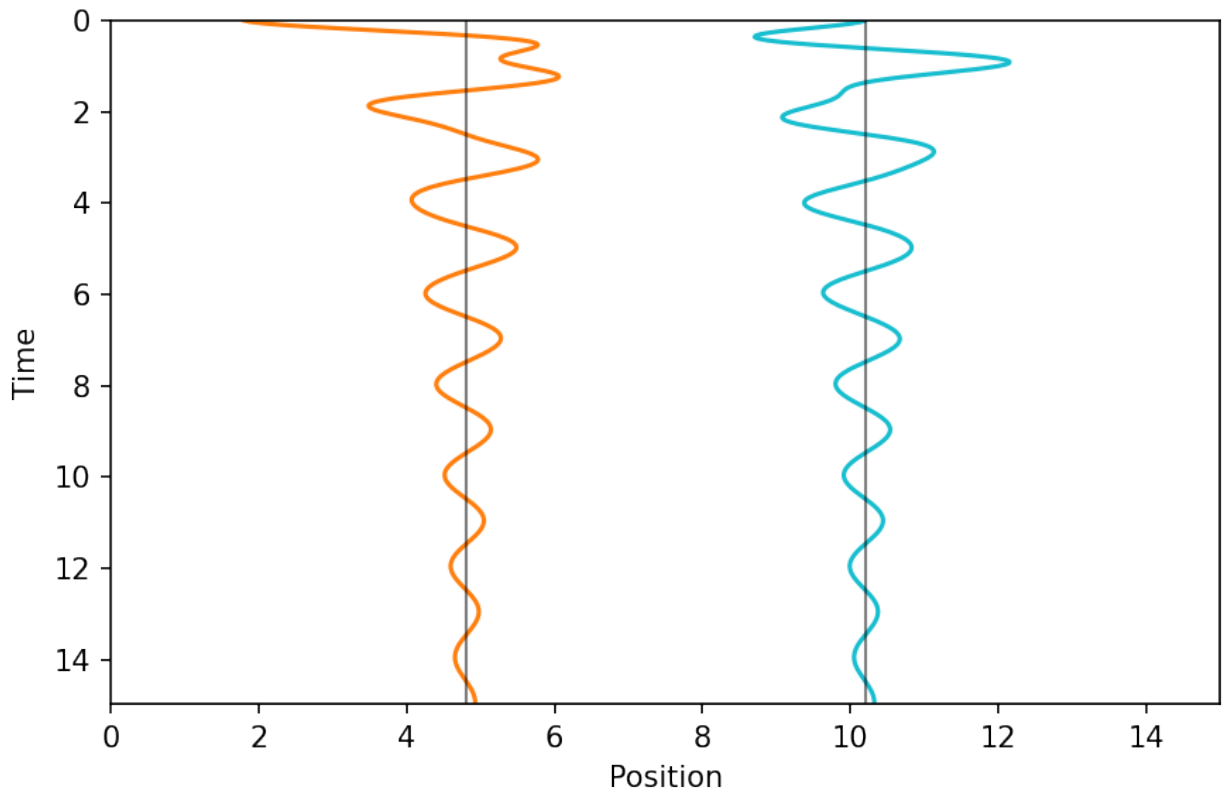
```
    fig.tight_layout()
    plt.show()
```

[38]:
```
plot_oszillations(data)
```



[39]:
```
from matplotlib import animation
from IPython.display import HTML
```

[40]:
```
def plot_animation(data, bw):
    fig, ax = plt.subplots()
    ax.axis("off")
    ax.set_aspect(1.)
    l1, = ax.plot(data.b1.x, data.t-data.t[0], c="C1", lw=1, zorder=-1)
    l2, = ax.plot(data.b2.x, data.t-data.t[0], c="C9", lw=1, zorder=-1)
    rectl = patches.Rectangle((-bw, -4.*bw), bw, 8.*bw, linewidth=1, edgecolor="#000000",
↪ facecolor="#dddddd", hatch="//")
    ax.add_patch(rectl)
    rectr = patches.Rectangle((L, -4.*bw), bw, 8.*bw, linewidth=1, edgecolor="#000000",␣
↪facecolor="#dddddd", hatch="//")
    ax.add_patch(rectr)
    ax.set_xlim(-2.*bw, L+2.*bw)
    ax.set_ylim(-5., 5.)
    b1 = patches.Circle((data.b1.x[0], 0), bw, linewidth=1, edgecolor="#000000",␣
↪facecolor="C1")
    ax.add_patch(b1)
```

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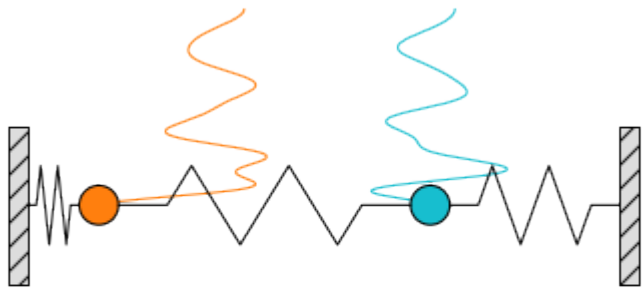
```
    b2 = patches.Circle((data.b2.x[0], 0), bw, linewidth=1, edgecolor="#000000",␣
↪facecolor="C9")
    ax.add_patch(b2)
    x, y = getspring(0., data.b1.x[0]-bw, bw)
    s1, = ax.plot(x, y, c="#000000", lw=1)
    x, y = getspring(data.b1.x[0]+bw, data.b2.x[0]-bw, bw)
    s2, = ax.plot(x, y, c="#000000", lw=1)
    x, y = getspring(data.b2.x[0]+bw, L, bw)
    s3, = ax.plot(x, y, c="#000000", lw=1)
    return fig, ax, l1, l2, b1, b2, s1, s2, s3
```

[41]:
```
def init():
    l1.set_data(data.b1.x, data.t-data.t[0])
    l2.set_data(data.b2.x, data.t-data.t[0])
    b1.center = (data.b1.x[0], 0.)
    ax.add_patch(b1)
    b2.center = (data.b2.x[0], 0.)
    ax.add_patch(b2)
    x, y = getspring(0., data.b1.x[0]-bw, bw)
    s1.set_data(x, y)
    x, y = getspring(data.b1.x[0]+bw, data.b2.x[0]-bw, bw)
    s2.set_data(x, y)
    x, y = getspring(data.b2.x[0]+bw, L, bw)
    s3.set_data(x, y)
    plt.show()
    return l1, l2, b1, b2, s1, s2, s3
```

[42]:
```
def animate(i):
    l1.set_data(data.b1.x, data.t-data.t[i])
    l2.set_data(data.b2.x, data.t-data.t[i])
    b1.center = (data.b1.x[i], 0.)
    b2.center = (data.b2.x[i], 0.)
    x, y = getspring(0., data.b1.x[i]-bw, bw)
    s1.set_data(x, y)
    x, y = getspring(data.b1.x[i]+bw, data.b2.x[i]-bw, bw)
    s2.set_data(x, y)
    x, y = getspring(data.b2.x[i]+bw, L, bw)
    s3.set_data(x, y)
    return l1, l2, b1, b2, s1, s2, s3
```

[43]:
```
fig, ax, l1, l2, b1, b2, s1, s2, s3 = plot_animation(data, 0.5)
```



[44]:
```
anim = animation.FuncAnimation(fig, animate, init_func=init,
                               frames=len(data.t), interval=1.e3/fps, blit=True)
```

[45]:
```
HTML(anim.to_html5_video())
```

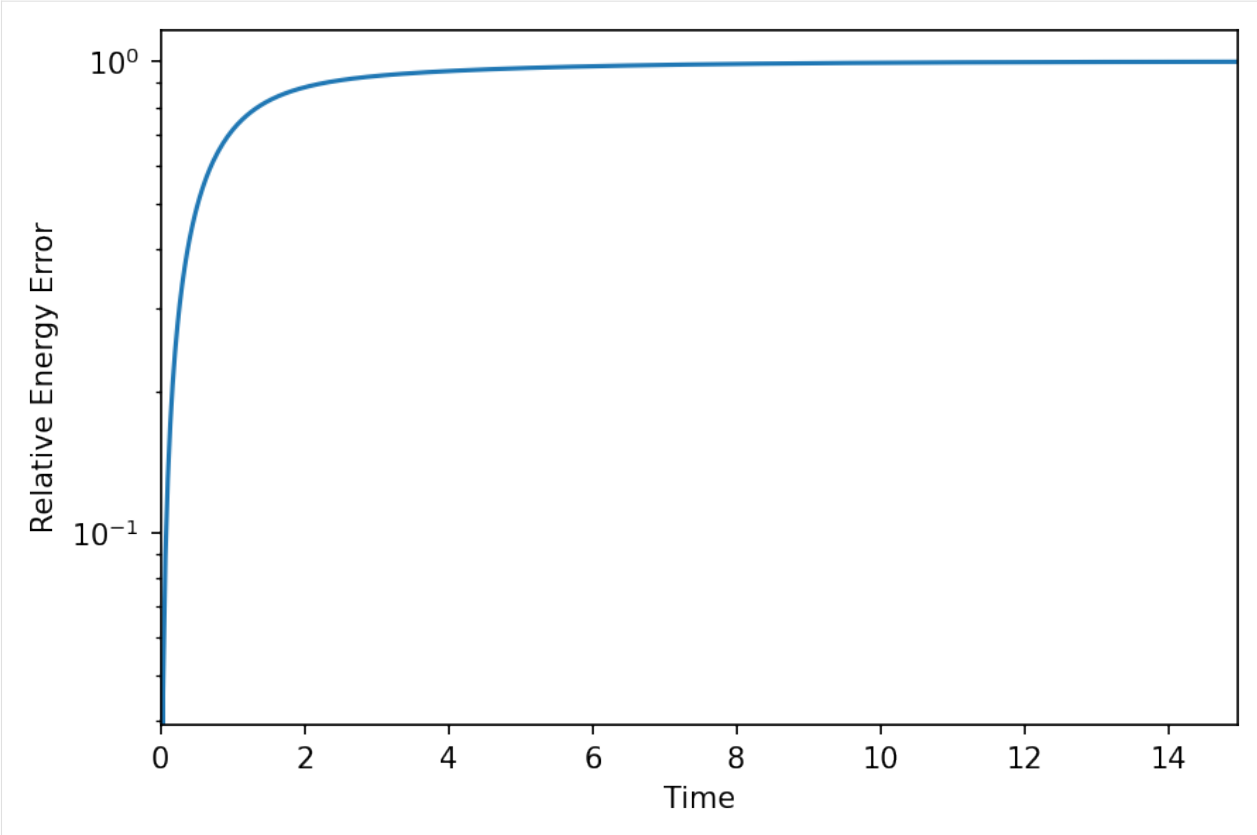
[45]:
```
<IPython.core.display.HTML object>
```

As you can see the oscillation is damped pretty quickly, which is weird because we did not include any damping term into our differential equations for the velocities.

We can plot the maximum relative error of the total energy in the system.

[46]:
```
def plot_energy(data):
    T = 0.5*(data.b1.m*data.Y[:, 2]**2 + data.b2.m*data.Y[:, 3]**2)
    V = 0.5*(data.s1.k*data.Y[:, 0]**2 + data.s2.k*(data.Y[:, 1]-data.Y[:, 0])**2 + data.
↪s3.k*data.Y[:, 1]**2)
    E = T + V
    dE = np.abs(E-E[0])/E[0]
    fig, ax = plt.subplots(dpi=150)
    ax.semilogy(data.t, dE)
    ax.set_xlabel("Time")
    ax.set_ylabel("Relative Energy Error")
    ax.set_xlim(data.t[0], data.t[-1])
    fig.tight_layout()
    plt.show()
```

[47]:
```
plot_energy(data)
```



The damping is purely numerically. The cause for the damping is the implicit integrator scheme used here, that is not suited for the problem, similar to the explicit integrator used for the orbital integration.

The implicit midpoint method is simplectic, i.e., energy conserving. We can use this instead.

Resetting

[48]:
```
sim.Y = (-3., 0., 0., 0)
sim.update()
sim.t = 0
sim.writer.reset()
```

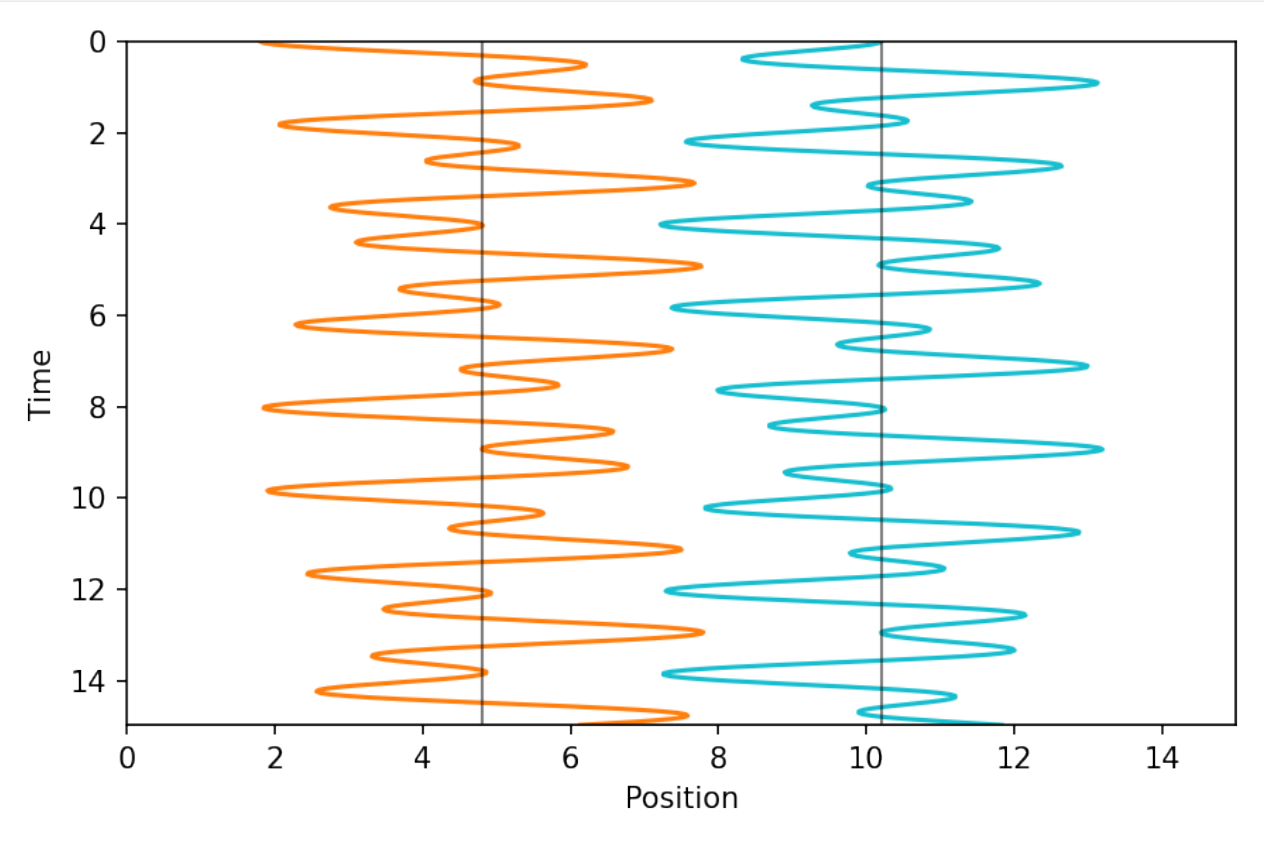
[49]:
```
sim.integrator.instructions = [Instruction(schemes.impl_2_midpoint_direct, sim.Y)]
```

[50]:
```
sim.run()
```

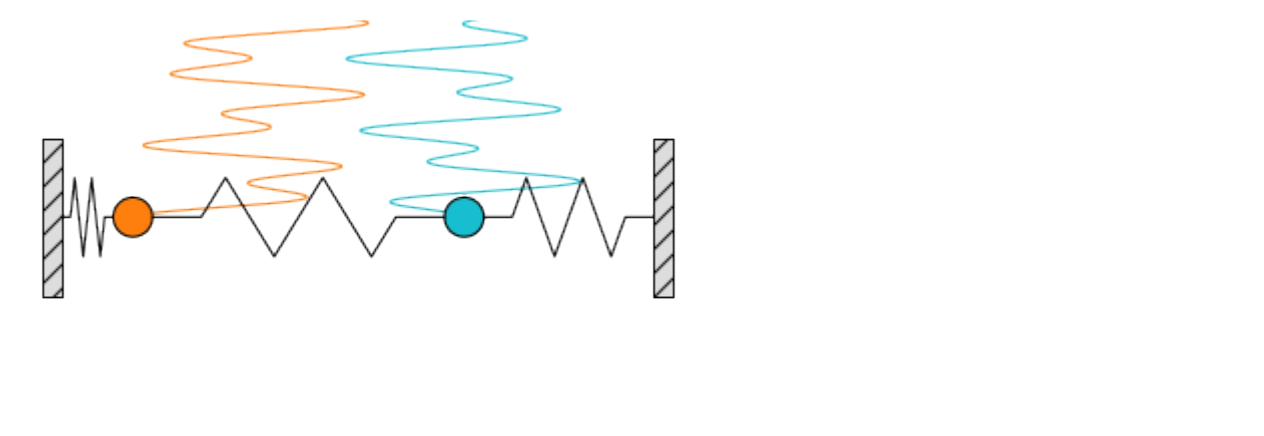
```
Execution time: 0:00:01
```

[51]:
```
data = sim.writer.read.all()
```

[52]:
```
plot_oszillations(data)
```



[53]:
```
fig, ax, l1, l2, b1, b2, s1, s2, s3 = plot_animation(data, 0.5)
```



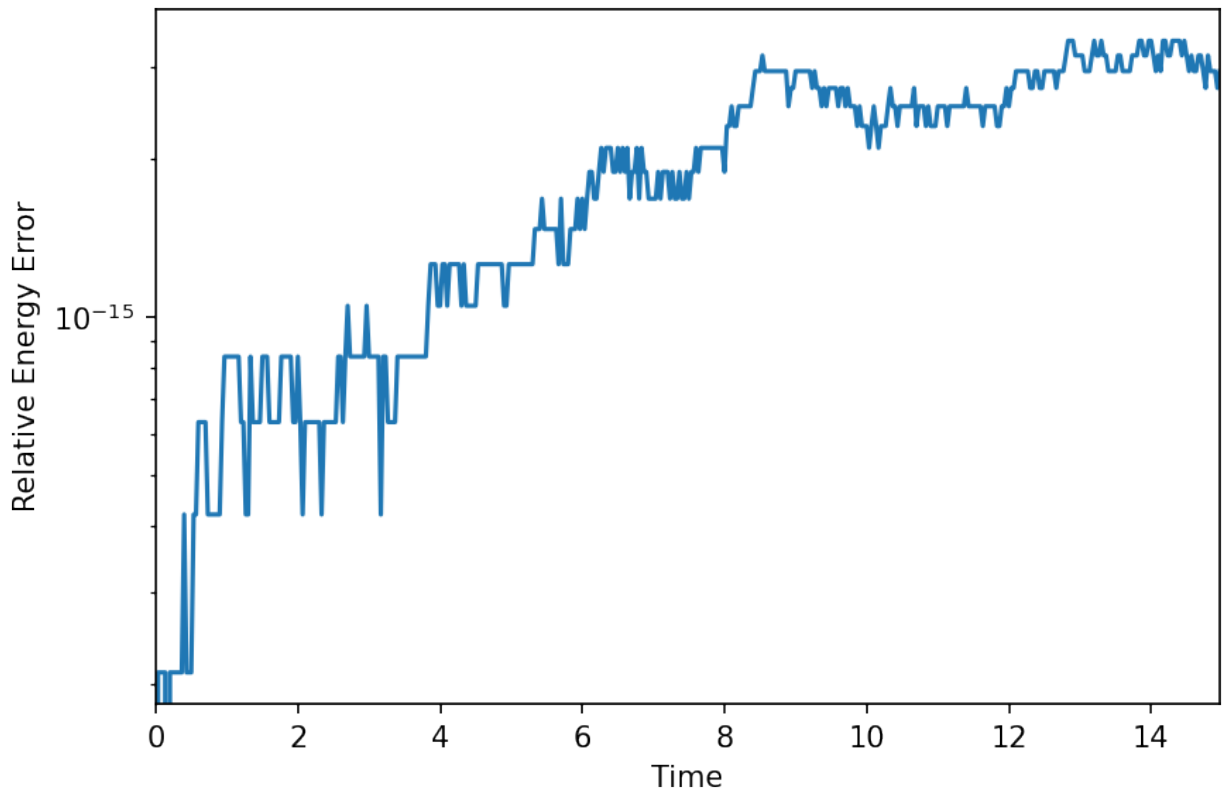
[54]:
```
anim = animation.FuncAnimation(fig, animate, init_func=init,
                               frames=len(data.t), interval=1.e3/fps, blit=True)
```

[55]:
```
HTML(anim.to_html5_video())
```

[55]:
```
<IPython.core.display.HTML object>
```

Now the damping is gone. The energy conservation plot now reads.

[56]:
```
plot_energy(data)
```



The energy error is of the order of the machine precision error.

But we could also easily use an explicit scheme. For explicit integration, we do not have to set the differentiator, since we have set a Jacobian and `simframe` is automatically calculating the derivative from the Jacobian.

Resetting

[57]:
```
sim.Y = (-3., 0., 0., 0)
sim.update()
sim.t = 0
sim.writer.reset()
```

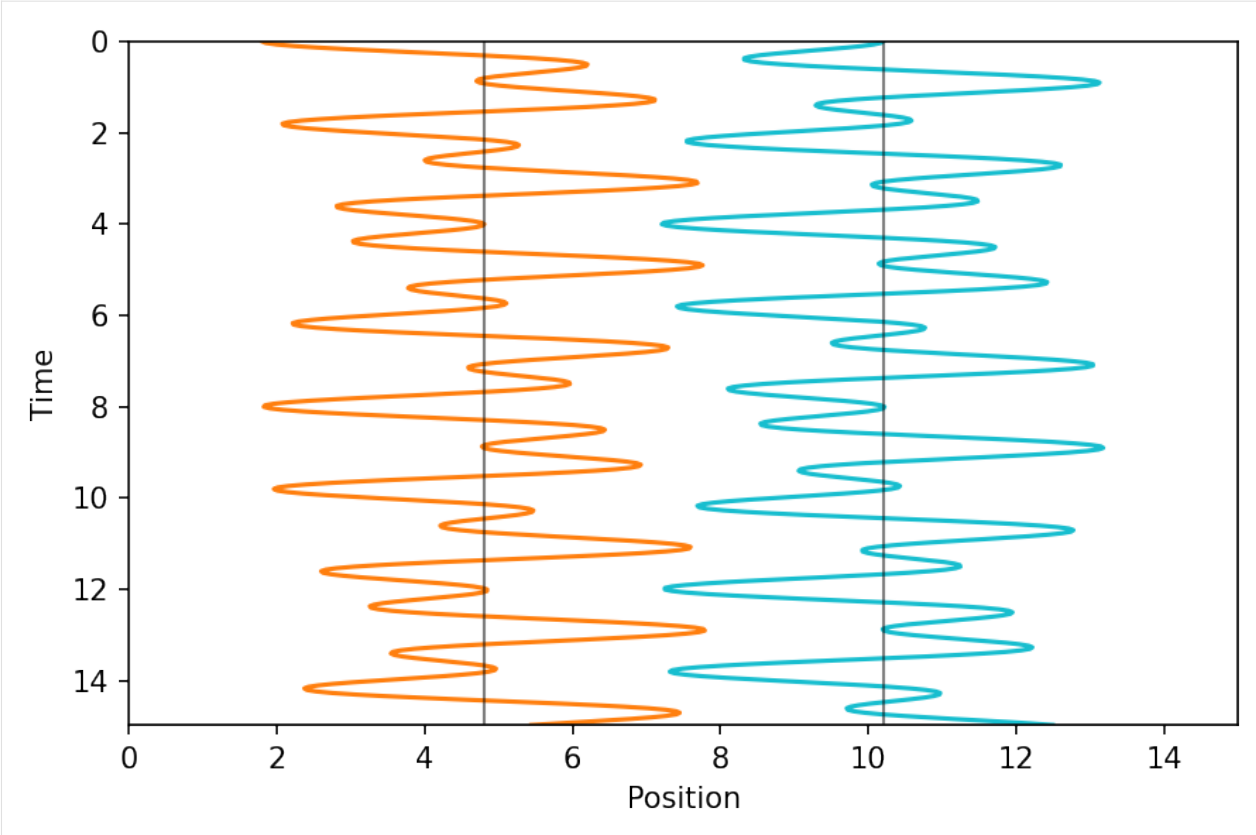
[58]:
```
sim.integrator.instructions = [Instruction(schemes.expl_4_runge_kutta, sim.Y)]
```

[59]:
```
sim.run()
```

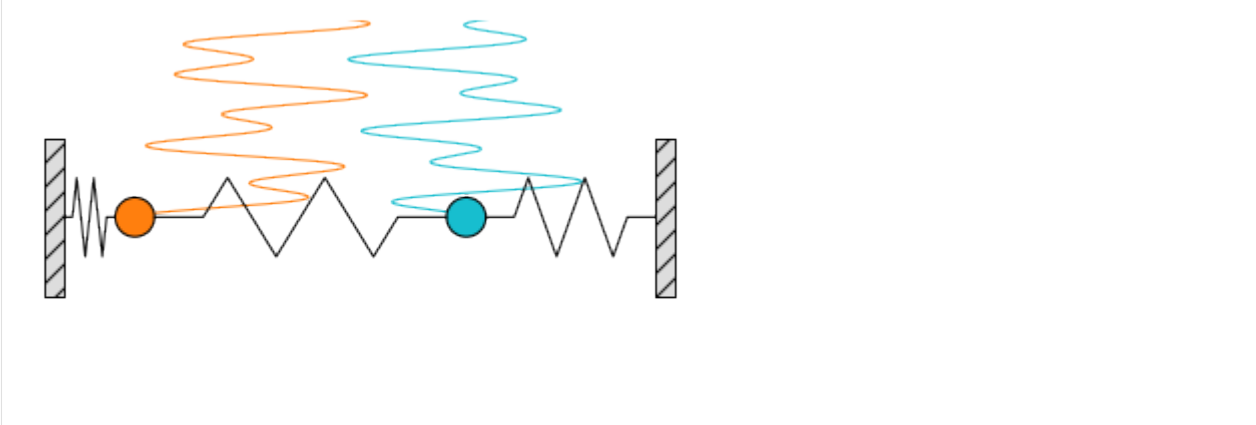
```
Execution time: 0:00:01
```

[60]:
```
data = sim.writer.read.all()
```

[61]:
```
plot_oszillations(data)
```



[62]:
```
fig, ax, l1, l2, b1, b2, s1, s2, s3 = plot_animation(data, 0.5)
```

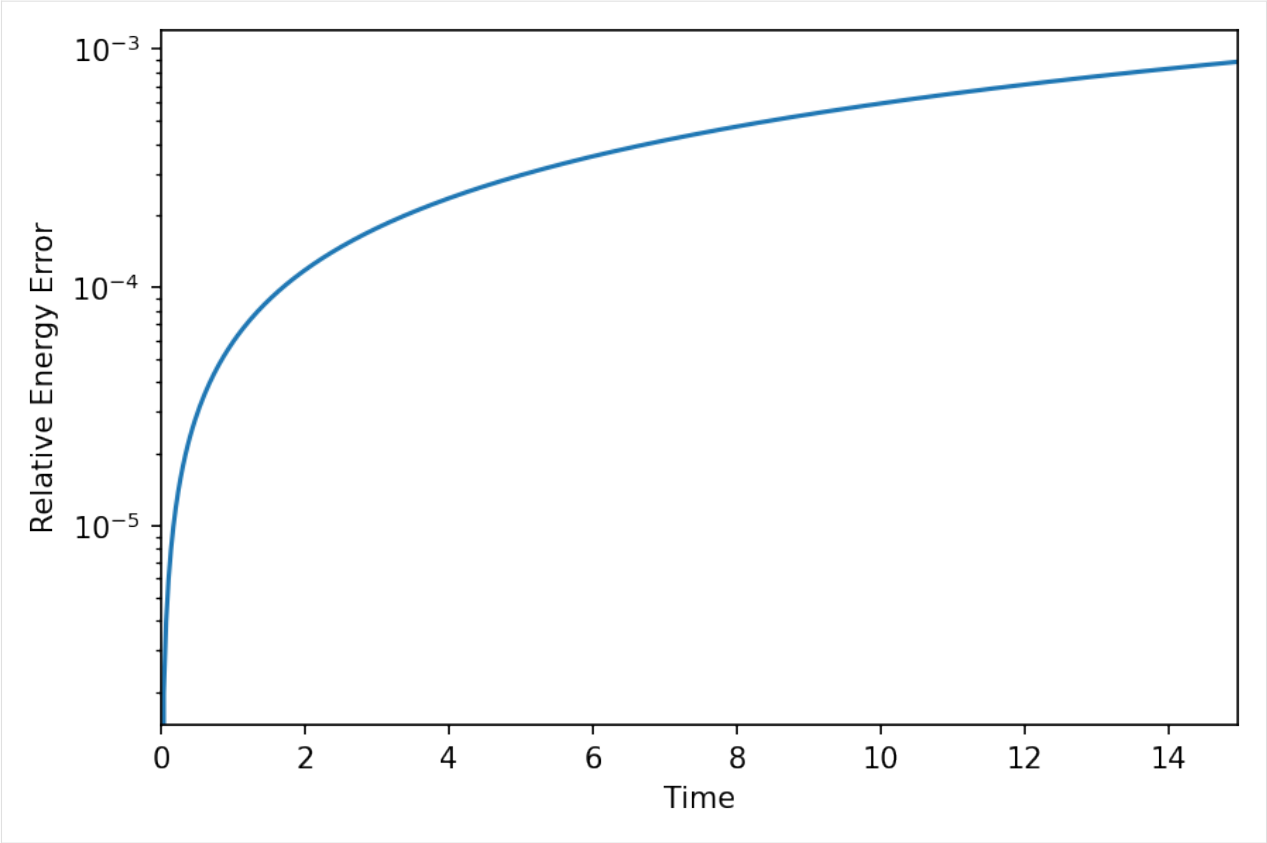


[63]:
```
anim = animation.FuncAnimation(fig, animate, init_func=init,
                               frames=len(data.t), interval=1.e3/fps, blit=True)
```

[64]:
```
HTML(anim.to_html5_video())
```

[64]:
```
<IPython.core.display.HTML object>
```

[65]:
```
plot_energy(data)
```



Here the energy error larger than for the symplectic scheme, but still smaller than in the first try.

CHAPTER

EIGHT

EXAMPLE: DOUBLE PENDULUM

In this example we are going to simulate the double pendulum with an adaptive integration scheme.

The double pendulum is two pendulums attached to each other with masses m_1 and m_2 and lengths l_1 and l_2. It is fully defined by two angles θ_1 and θ_2 and two angular velocities $\omega_1 = \dot{\theta}_1$ and $\omega_2 = \dot{\theta}_2$. We are therefore going to simulate the evolution of the state vector

$$\vec{Y} = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \omega_1 \\ \omega_2 \end{pmatrix}$$

[1]:
```
# Mass and length of 1st pendulum
mass1 = 1.
length1 = 1.
# Mass and length of 2nd pendulum
mass2 = 1.
length2 = 2.
```

We are going to store the quantities of the two pendulums in separate groups.

[2]:
```
from simframe import Frame
```

[3]:
```
sim = Frame(description="Double Pendulum")
```

[4]:
```
sim.addgroup("p1", description="Pendulum 1")
sim.addgroup("p2", description="Pendulum 2")
```

[5]:
```
sim.p1.addfield("m", mass1, description="Mass", constant=True)
sim.p1.addfield("l", length1, description="Length", constant = True)
sim.p1.addfield("r", [0., 0.], description="Cartesian position vector")

sim.p2.addfield("m", mass2, description="Mass", constant=True)
sim.p2.addfield("l", length2, description="Length", constant = True)
sim.p2.addfield("r", [0., 0.], description="Cartesian position vector")
```

And we create a field for the state vector and initialize it with some values for the angles.

[6]:
```
import numpy as np
```

[7]:
```
Y0 = [
    0.25*np.pi, # theta 1
```

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```
    0.15*np.pi, # theta 2
    0.,         # omega 1
    0.          # omega 2
]
```

[8]:
```
sim.addfield("Y", Y0, description="State vector")
```

For convenience we store the cartesian coordinates of the masses in their respective groups. Therefore we need functions that convert the angles into cartesian coordinates and assign it to their updaters.

$$\vec{r}_1 = \begin{pmatrix} l_1 \sin\theta_1 \\ -l_1 \cos\theta_1 \end{pmatrix}$$

$$\vec{r}_2 = \begin{pmatrix} l_1 \sin\theta_1 + l_2 \sin\theta_2 \\ -l_1 \cos\theta_1 - l_2 \cos\theta_2 \end{pmatrix}$$

[9]:
```
def r1(sim):
    theta1 = sim.Y[0]
    theta2 = sim.Y[1]
    return sim.p1.l*np.sin(theta1), -sim.p1.l*np.cos(theta1)

def r2(sim):
    theta1 = sim.Y[0]
    theta2 = sim.Y[1]
    return sim.p1.l*np.sin(theta1)+sim.p2.l*np.sin(theta2), -sim.p1.l*np.cos(theta1)-sim.
↪p2.l*np.cos(theta2)
```

[10]:
```
sim.p1.r.updater = r1
sim.p2.r.updater = r2
```

Now we have to assign updaters to the group and the simulation object.

[11]:
```
sim.p1.updater = ["r"]
sim.p2.updater = ["r"]
sim.updater = ["p1", "p2"]
```

After updating the simulation frame, the cartesian coordinates are stored in the pendulum groups.

[12]:
```
sim.update()
```

[13]:
```
print("x1 = {:4.1f}, y1 = {:4.1f}\nx2 = {:4.1f}, y2 = {:4.1f}".format(sim.p1.r[0], sim.
↪p1.r[1], sim.p2.r[0], sim.p2.r[1]))
```

```
x1 =  0.7, y1 = -0.7
x2 =  1.6, y2 = -2.5
```

Here is a plot to visualize the problem.

[14]:
```
import matplotlib.pyplot as plt
import matplotlib.patches as patches
```

[15]:
```
def plot_system(sim):
    fig = plt.figure(dpi=150)
```

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```
    ax = fig.add_subplot(111, aspect=1.)
    ax.axis("off")

    # Maximum radius the double pendulum can have
    L = sim.p1.l + sim.p2.l
    # Radius of a ball in the plot
    r = 0.05*L

    p1 = patches.Circle(sim.p1.r, r, linewidth=1, edgecolor="#000000", facecolor="C1")
    ax.add_patch(p1)
    p2 = patches.Circle(sim.p2.r, r, linewidth=1, edgecolor="#000000", facecolor="C9")
    ax.add_patch(p2)
    circ = patches.Circle((0, 0), sim.p1.l, linewidth=1, edgecolor="C1", facecolor="None
↪", zorder=-1, ls="--")
    ax.add_patch(circ)
    origin = patches.Circle((0, 0), 0.5*r, linewidth=1, edgecolor=None, facecolor="C3")
    ax.add_patch(origin)

    ax.plot([0, sim.p1.r[0]], [0, sim.p1.r[1]], zorder=-1, lw=1, c="#000000")
    ax.plot([sim.p2.r[0], sim.p1.r[0]], [sim.p2.r[1], sim.p1.r[1]], zorder=-1, lw=1, c="
↪#000000")

    ax.set_xlim(-1.1*L, 1.1*L)
    ax.set_ylim(-1.1*L, 1.1*L)

    fig.tight_layout()

    return fig, ax
```

[16]:
```
fig, ax = plot_system(sim)

L = sim.p1.l + sim.p2.l
r = 0.05*L

theta1 = patches.Wedge([0, 0], 0.75*sim.p1.l, -90, sim.Y[0]/np.pi*180.-90, linewidth=0.5,
↪ edgecolor="#000000", facecolor="None", zorder=-1)
ax.add_patch(theta1)
theta2 = patches.Wedge([sim.p1.r[0], sim.p1.r[1]], 0.75*sim.p2.l, -90, sim.Y[1]/np.
↪pi*180.-90, linewidth=0.5, edgecolor="#000000", facecolor="None", zorder=-1)
ax.add_patch(theta2)

ax.text(sim.p1.r[0], sim.p1.r[1], "$m_1$", ha="center", va="center", fontsize="x-small")
ax.text(sim.p2.r[0], sim.p2.r[1], "$m_2$", ha="center", va="center", fontsize="x-small")
ax.text(0.5*sim.p1.r[0]+r, 0.5*sim.p1.r[1]+r, "$l_1$", ha="center", va="center")
ax.text(0.5*(sim.p1.r[0]+sim.p2.r[0])+r, 0.5*(sim.p1.r[1]+sim.p2.r[1])+r, "$l_2$", ha=
↪"center", va="center")

ax.text(0.5*sim.p1.l*np.sin(0.5*sim.Y[0]), -0.5*sim.p1.l*np.cos(0.5*sim.Y[0]), r"$\theta_
↪1$", ha="center", va="center")
ax.text(0.5*sim.p2.l*np.sin(0.5*sim.Y[1])+sim.p1.r[0], -0.5*sim.p2.l*np.cos(0.5*sim.
↪Y[1])+sim.p1.r[1], r"$\theta_2$", ha="center", va="center")
```

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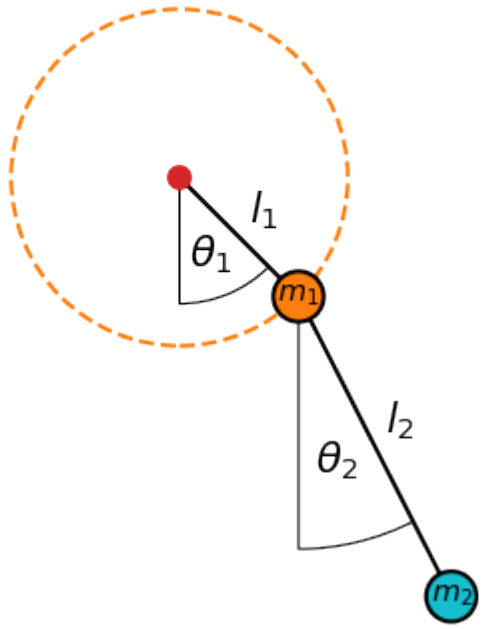
```
plt.show()
```



We now need the equations of motion of the problem. We are going to use Lagrangian mechanics to get the derivates of ω_1 and ω_2.

The kinetic energy of the system is given by

$T = \frac{1}{2}m_1 v_1^2 + \frac{1}{2}m_2 v_2^2 = \frac{1}{2}m_1\left(\dot{x}_1^2 + \dot{y}_1^2\right) + \frac{1}{2}m_2\left(\dot{x}_2^2 + \dot{y}_2^2\right)$

From the definition of the cartesian coordinates above we get

$\dot{x}_1 = l_1\omega_1\cos\theta_1, \quad \dot{y}_1 = l_1\omega_1\sin\theta_1$

$\dot{x}_2 = l_1\omega_1\cos\theta_1 + l_2\omega_2\cos\theta_2, \quad \dot{y}_2 = l_1\omega_1\sin\theta_1 + l_2\omega_2\sin\theta_2$

which yields

$T = \frac{1}{2}m_1 l_1^2\omega_1^2 + \frac{1}{2}m_2\left(l_1^2\omega_1^2 + l_2^2\omega_2^2 + 2l_1 l_2\omega_1\omega_2\cos\left(\theta_1 - \theta_2\right)\right),$

where $\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2 = \cos(\theta_1 - \theta_2)$ was used.

The potential energy of the system is given by

$V = gm_1y_1 + gm_2y_2 = -g(m_1+m_2)\,l_1\cos\theta_1 - gm_2l_2\cos\theta_2$

with the gravitational acceleration g.

Therefore, the Langrangian is given by

$\mathcal{L} = T - V = \frac{1}{2}m_1l_1^2\omega_1^2 + \frac{1}{2}m_2\left(l_1^2\omega_1^2 + l_2^2\omega_2^2 + 2l_1l_2\omega_1\omega_2\cos(\theta_1-\theta_2)\right) + g(m_1+m_2)\,l_1\cos\theta_1 + gm_2l_2\cos\theta_2$

The canonical momenta conjugate to θ_i are given by

$p_{\theta_i} = \frac{\partial\mathcal{L}}{\partial\dot{\theta}_i}$

These are

$p_{\theta_1} = \frac{\partial\mathcal{L}}{\partial\omega_1} = (m_1+m_2)\,l_1^2\omega_1 + m_2l_1l_2\omega_1\cos(\theta_1-\theta_2)$

$p_{\theta_2} = \frac{\partial\mathcal{L}}{\partial\omega_2} = m_2l_2^2\omega_2 + m_2l_1l_2\omega_1\cos(\theta_1-\theta_2)$

The Euler-Lagrange equations of motion are given by

$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\mathcal{L}}{\partial\omega_i}\right) - \frac{\partial\mathcal{L}}{\partial\theta_i} = 0,$

which are a set of two coupled differential equations in the case of the double pendulum, that can be simplified to

$\dot{\omega}_1 + \frac{m_2}{m_1+m_2}\frac{l_2}{l_1}\cos(\theta_1-\theta_2)\,\dot{\omega}_2 = -\frac{m_2}{m_1+m_2}\frac{l_2}{l_1}\omega_2^2\sin(\theta_1-\theta_2) - \frac{g}{l_1}\sin\theta_1$

$\frac{l_1}{l_2}\cos(\theta_1-\theta_2)\,\dot{\omega}_1 + \dot{\omega}_2 = \frac{l_1}{l_2}\omega_1^2\sin(\theta_1-\theta_2) - \frac{g}{l_2}\sin\theta_1$

This system of equations can be written as a matrix equation

$\mathbb{A}\cdot\begin{pmatrix}\dot{\omega}_1\\ \dot{\omega}_2\end{pmatrix} = \begin{pmatrix}1 & \alpha_1\\ \alpha_2 & 1\end{pmatrix}\cdot\begin{pmatrix}\dot{\omega}_1\\ \dot{\omega}_2\end{pmatrix} = \begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix}.$

This matrix equation can be solved for $\dot{\omega}_1$ and $\dot{\omega}_2$ via

$\begin{pmatrix}\dot{\omega}_1\\ \dot{\omega}_2\end{pmatrix} = \mathbb{A}^{-1}\cdot\begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix}$

Since the determinant of $\mathbb{A}$ always differs from zero

$\det\mathbb{A} = 1 - \alpha_1\alpha_2 = 1 - \frac{m_2}{m_1+m_2}\cos^2(\theta_1-\theta_2) \neq 0$

the matrix itself can always be inverted.

$\mathbb{A}^{-1} = \frac{1}{\det\mathbb{A}}\begin{pmatrix}1 & -\alpha_1\\ -\alpha_2 & 1\end{pmatrix}$

Therefore, the equations of motion for ω_1 and ω_2 are given by

$\dot{\omega}_1 = \frac{\beta_1-\alpha_1\beta_2}{1-\alpha_1\alpha_2}$

$\dot{\omega}_2 = \frac{\beta_2-\alpha_2\beta_1}{1-\alpha_1\alpha_2}$

We can now write a function that returns the derivate of our state vector $\vec{Y}$.

[17]:
```
# Gravitational acceleration in m/s²
g = 9.81
```

[18]:
```
def dYdt(sim, x, Y):
    theta1 = Y[0]
    theta2 = Y[1]
```

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```
    omega1 = Y[2]
    omega2 = Y[3]

    # Derivatives of the angles
    dtheta1 = omega1
    dtheta2 = omega2

    beta1 = -sim.p2.m/(sim.p1.m+sim.p2.m)*sim.p2.l/sim.p1.l*omega2**2*np.sin(theta1-
↪theta2) - g/sim.p1.l*np.sin(theta1)
    beta2 = sim.p1.l/sim.p2.l*omega1**2*np.sin(theta1-theta2) - g/sim.p2.l*np.sin(theta2)

    alpha1 = sim.p2.m/(sim.p1.m+sim.p2.m)*sim.p2.l/sim.p1.l*np.cos(theta1-theta2)
    alpha2 = sim.p1.l/sim.p2.l*np.cos(theta1-theta2)
    detA = 1. - alpha1*alpha2

    # Derivatives of the angular velocities
    domega1 = (beta1-alpha1*beta2)/detA
    domega2 = (beta2-alpha2*beta1)/detA

    return np.array([dtheta1, dtheta2, domega1[0], domega2[0]])
```

This function has to be assigned to the differentiator of the state vector.

[19]:
```
sim.Y.differentiator = dYdt
```

Now we can set up the integration variable.

[20]:
```
sim.addintegrationvariable("t", 0., description="Time")
```

Since we are going to use an adaptive scheme, the timestep we want to use is the timestep suggested by the scheme.

[21]:
```
def dt(sim):
    return sim.t.suggested
```

[22]:
```
sim.t.updater = dt
```

We have to suggest a timestep initially for the scheme to work.

[23]:
```
sim.t.suggest(1.)
```

We want to create an animation later from the simulation result. Therefore, we define the snapshots in a way that they match our desired frame rate. For this we define the frames per second and the maximum simulation time.

[24]:
```
fps = 30.
t_max = 30.
```

[25]:
```
sim.t.snapshots = np.arange(1./fps, t_max, 1./fps)
```

Next we can set up the integrator.

[26]:
```
from simframe import Integrator
from simframe import Instruction
from simframe import schemes
```

[27]:
```
sim.integrator = Integrator(sim.t)
```

We have one integration instruction that is integrating our state vector with the 5th-order adaptive Cash-Karp scheme. We also lower the value of ϵ, which is the maximum accepted relative error of the integration scheme.

[28]:
```
sim.integrator.instructions = [
    Instruction(schemes.expl_5_cash_karp_adptv, sim.Y, controller={"eps": 0.001})
]
```

We do not want to write output files. Instead we use the namespace writer to store the data in the simulation frame itself.

[29]:
```
from simframe import writers
```

[30]:
```
sim.writer = writers.namespacewriter()
```

Since we are having many snapshots we do not want the writer to write on screen.

[31]:
```
sim.writer.verbosity = 0
```

For a more interesting example we change the initial conditions.

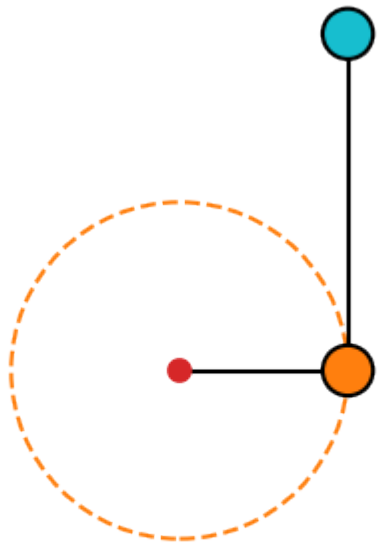
[32]:
```
Y0 = [
    0.5*np.pi,  # theta 1
    1.0*np.pi,  # theta 2
    0.,         # omega 1
    0.          # omega 2
]
```

[33]:
```
sim.Y[:] = Y0
```

[34]:
```
sim.update()
```

We can now plot the initial state.

[35]:
```
fig, ax = plot_system(sim)
```



We are now ready to run the simulation.

[36]:
```
sim.run()
```

```
Execution time: 0:00:18
```

After the simulation is finished we can read the data

[37]:
```
data = sim.writer.read.all()
```

and plot the trajectory of the second pendulum.

[38]:
```
def plot_trajectories(dataset):
    fig, ax = plt.subplots(dpi=150.)
    ax.set_aspect(1.)
    ax.axis("off")
```

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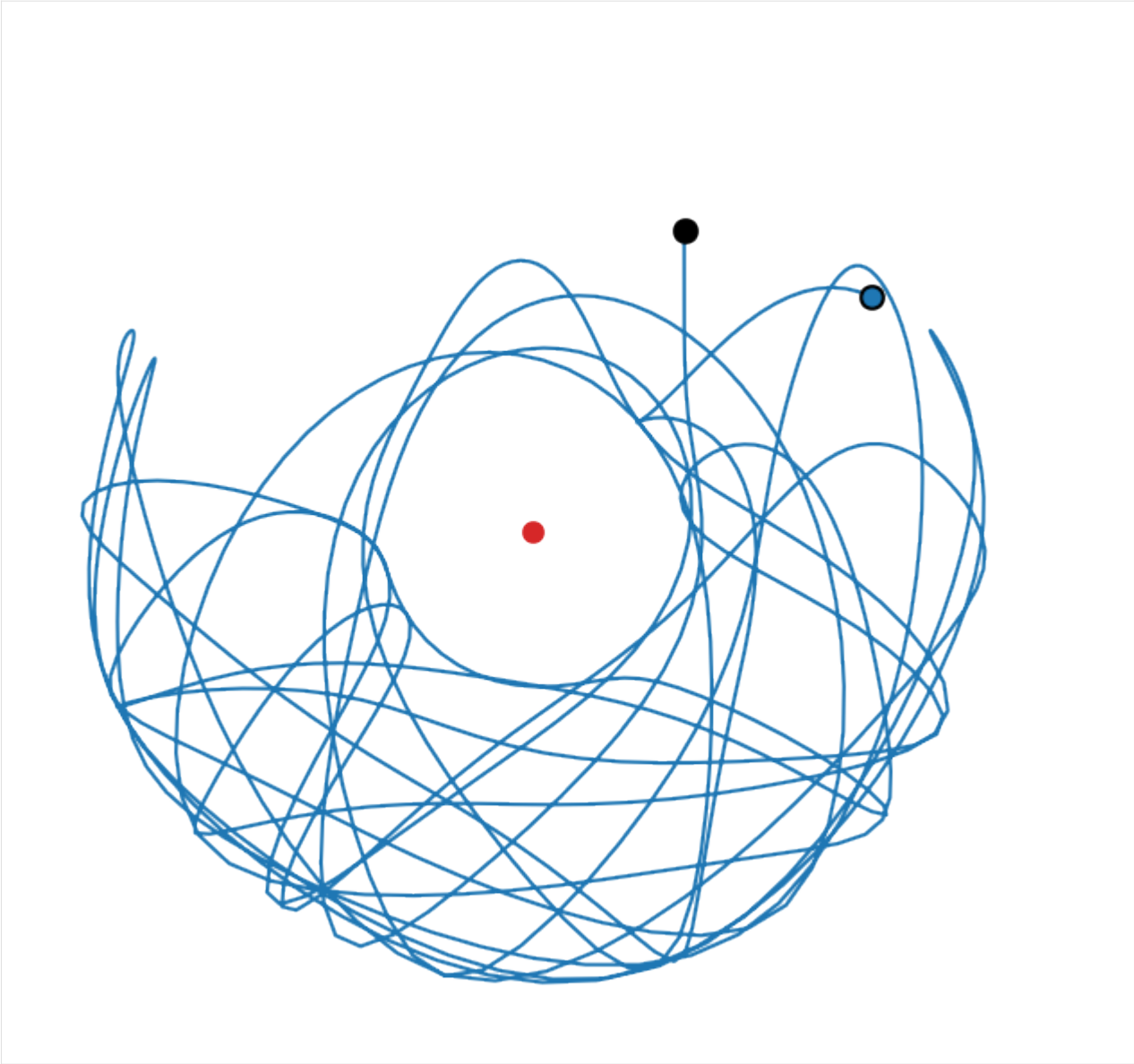
```
    L = dataset[0].p1.l[0] + dataset[0].p2.l[0]
    r = 0.05*L

    origin = patches.Circle((0, 0), 0.5*r, linewidth=1, edgecolor=None, facecolor="C3")
    ax.add_patch(origin)

    for d in dataset:
        p, = ax.plot(d.p2.r[:, 0], d.p2.r[:, 1], lw=1, zorder=-1)
        ax.plot(d.p2.r[-1, 0], d.p2.r[-1, 1], "o", c=p.get_color(), markeredgecolor="
↪#000000")
        ax.plot(d.p2.r[0, 0], d.p2.r[0, 1], "o", c="#000000")

    ax.set_xlim(-1.1*L, 1.1*L)
    ax.set_ylim(-1.1*L, 1.1*L)

    fig.tight_layout()
```

[39]:
```
plot_trajectories([data])
```



We should also check for energy conservation to see if the integration scheme was accurate enough.

[40]:
```
def plot_energy_error(data):
    vx1 = data.Y[:, 2]*data.p1.l*np.cos(data.Y[:, 0])
    vy1 = data.Y[:, 2]*data.p1.l*np.sin(data.Y[:, 0])
    vx2 = vx1 + data.Y[:, 3]*data.p2.l*np.cos(data.Y[:, 1])
    vy2 = vy1 + data.Y[:, 3]*data.p2.l*np.sin(data.Y[:, 1])
    v1 = np.sqrt(vx1**2+vy1**2)
    v2 = np.sqrt(vx2**2+vy2**2)
    T = 0.5*(data.p1.m*v1**2 + data.p2.m*v2**2)
    V = g*(data.p1.m*data.p1.r[:, 1] + data.p2.m*data.p2.r[:, 1])
    E = T+V
    fig, ax = plt.subplots(dpi=150.)
    ax.semilogy(data.t, np.abs(E-E[0])/E[0])
    ax.set_xlim(data.t[0], data.t[-1])
```

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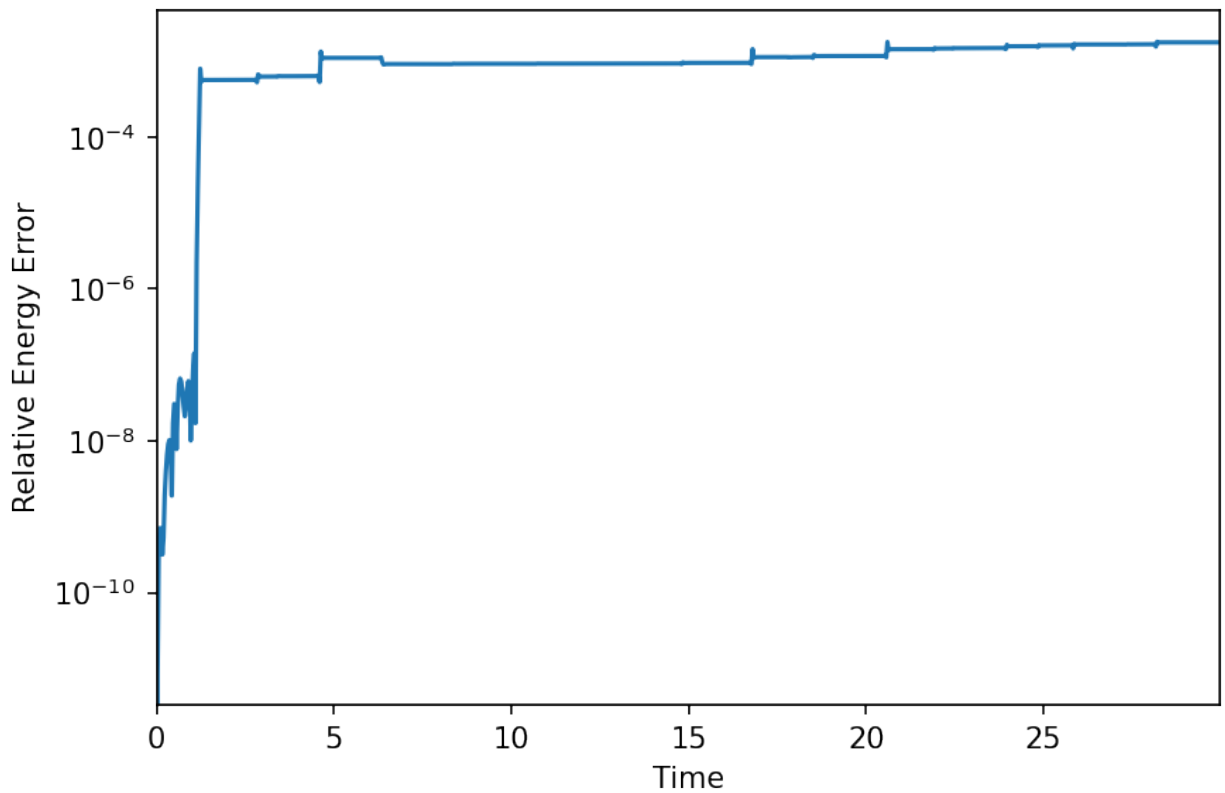
```
    ax.set_xlabel("Time")
    ax.set_ylabel("Relative Energy Error")
    fig.tight_layout()
```

[41]:
```
plot_energy_error(data)
```



The maximum relative energy error that we have in our simulation is less that 0.1%.

Note: we could have also used the leapfrog integrator as in the example of the coupled oscillators for better energy conservation.

We can also create an animation of the entire simulation.

[42]:
```
def plot_animation(data):
    fig = plt.figure()
    ax = fig.add_subplot(111, aspect=1.)
    ax.axis("off")

    L = sim.p1.l + sim.p2.l
    r = 0.05*L

    p1 = patches.Circle(data.p1.r[0], r, linewidth=1, edgecolor="#000000", facecolor="C1
↪")
    ax.add_patch(p1)
    p2 = patches.Circle(data.p2.r[0], r, linewidth=1, edgecolor="#000000", facecolor="C9
↪")
```

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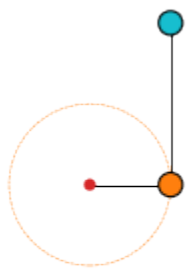
```
    ax.add_patch(p2)
    circ = patches.Circle((0, 0), data.p1.l[0], linewidth=1, edgecolor="C1", facecolor=
↪"None", zorder=-1, ls="--", lw=0.5)
    ax.add_patch(circ)
    origin = patches.Circle((0, 0), 0.5*r, linewidth=1, edgecolor=None, facecolor="C3")
    ax.add_patch(origin)

    l1, = ax.plot([0, data.p1.r[0, 0]], [0, data.p1.r[0, 1]], zorder=-1, lw=1, c="#000000
↪")
    l2, = ax.plot([data.p2.r[0, 0], data.p1.r[0, 0]], [data.p2.r[0, 1], data.p1.r[0, 1]],
↪ zorder=-1, lw=1, c="#000000")
    plot2, = ax.plot(data.p2.r[0, 0], data.p2.r[0, 1], c="C9", lw=0.1, alpha=0.5)

    ax.set_xlim(-1.1*L, 1.1*L)
    ax.set_ylim(-1.1*L, 1.1*L)

    fig.tight_layout()

    return fig, ax, p1, p2, l1, l2, plot2
```

[43]:
```
def init():
    p1.center = (data.p1.r[0])
    ax.add_patch(p1)
    p2.center = (data.p2.r[0])
    ax.add_patch(p2)
    l1.set_data([0, data.p1.r[0, 0]], [0, data.p1.r[0, 1]])
    l2.set_data([data.p2.r[0, 0], data.p1.r[0, 0]], [data.p2.r[0, 1], data.p1.r[0, 1]])
    plot2.set_data(data.p2.r[0, 0], data.p2.r[0, 1])
    plt.show()
    return p1, p2, l1, l2, plot2
```

[44]:
```
def animate(i):
    p1.center = (data.p1.r[i])
    p2.center = (data.p2.r[i])
    l1.set_data([0, data.p1.r[i, 0]], [0, data.p1.r[i, 1]])
    l2.set_data([data.p2.r[i, 0], data.p1.r[i, 0]], [data.p2.r[i, 1], data.p1.r[i, 1]])
    plot2.set_data(data.p2.r[:i, 0], data.p2.r[:i, 1])
    plt.show()
    return p1, p2, l1, l2, plot2
```

[45]:
```
fig, ax, p1, p2, l1, l2, plot2 = plot_animation(data)
```



[46]:
```
from matplotlib import animation
from IPython.display import HTML
```

[47]:
```
anim = animation.FuncAnimation(fig, animate, init_func=init,
                               frames=len(data.t), interval=1.e3/fps, blit=True)
```

[48]:
```
HTML(anim.to_html5_video())
```

[48]:
```
<IPython.core.display.HTML object>
```

The double pendulum is a chaotic system. With slightly different initial conditions, the result will differ drastically. We are now going to run the simulation again with slightly different initial conditions and compare the results.

[49]:
```
f_theta2 = [0.999, 1.001]
```

We are going to multiply the initial angle of the second pendulum by 0.999 and 1.001 and run the simulation again.

[50]:
```
def restart(sim, f_theta2):
    ret = []
    for f in f_theta2:
        sim.Y[:] = Y0
        sim.Y[1] *= f
        sim.update()
        sim.writer.reset()
        sim.t = 0.
        sim.run()
        data = sim.writer.read.all()
        ret.append(data)
    return ret
```

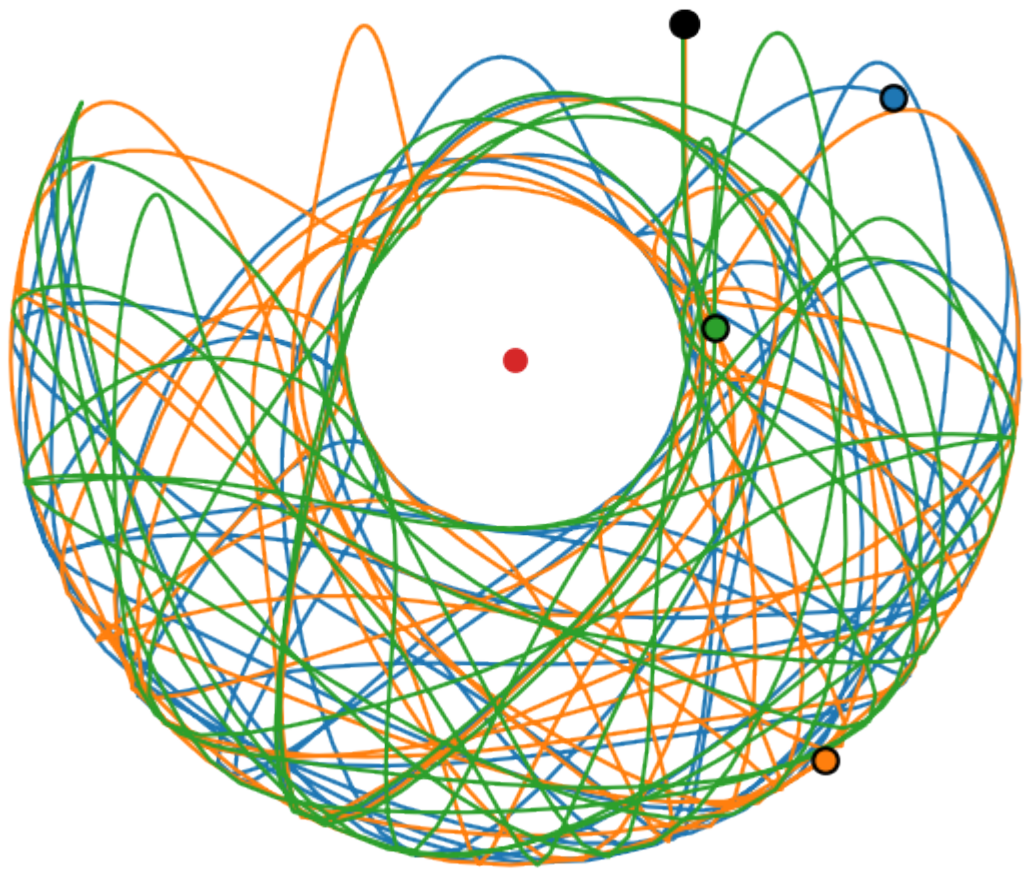
[51]:
```
data_new = restart(sim, f_theta2)
```

```
Execution time: 0:00:12
Execution time: 0:00:11
```

We combine the old and new results in one list and plot the trajectories of the second pendulum.

[52]:
```
data_new.insert(0, data)
```

[53]:
```
plot_trajectories(data_new)
```



Although all simulations started at almost the same spot, the final position of the second pendulum differs drastically.

CHAPTER

NINE

EXAMPLE: COMPARTMENTAL MODELS

In this notebook we are going to investigate compartmental models for infectious diseases.
In these models the entire population is divided into different compartments whose evolution is simulated over time.

In the first example we are going to create a simple compartmental model of a fictional disease and investigate how the compartments developed with time-dependent parameters.
In the second example we are going to run a more complex model of the SARS-CoV-2 outbreak.

9.1 SIRD Model

One of the simplest models is for example the SIRD model, which consists of four compartments: Susceptible, Infectious, Recovered, and Deceased. The four compartments are governed by the differential equations

$\frac{\mathrm{d}}{\mathrm{d}t} S = -\alpha R_1 \frac{SI}{N}$

$\frac{\mathrm{d}}{\mathrm{d}t} I = \alpha R_1 \frac{SI}{N} - (1-\beta) R_2 I - \beta R_3 I$

$\frac{\mathrm{d}}{\mathrm{d}t} R = (1-\beta)\, R_2 I$

$\frac{\mathrm{d}}{\mathrm{d}t} D = \beta R_3 I$

where R_1 is the average rate of contacts per person per time, α the probability of disease transmission per contact, β the mortality, R_2 the average recovery time, and R_3 the average time until death. $N = S + I + R + D$ is the total size of the population.

There are a few key parameters to describe the system. The basic reproduction number R_0 is the expected number of new infections if there is one infected person with the entire population susceptible. In our model this would be.

$R_0 = \frac{\alpha R_1}{\beta R_2 + (1-\beta) R_3}$

In general, the time-dependent reproduction number is the ratio of influx into the infectious comparments to the outflux from those compartments. In our model this is

$R_t = R_0 \frac{S}{N}$

To set up the model, we need to define the free parameters. We are going to assume that the population has a size of 10 million people. On average these people have 5 contacts per day. The transmission probability per contact of our fictitious disease it $5\,\%$. Of all infected $97\,\%$ will recover within 14 days, while $3\,\%$ will die within 14 days after infection. Initially we have one infected person: patient zero.

The base time unit of the model will be days.

[1]:
```
N     = 10_000_000.  # Total population size
alpha = 0.05         # Transmission probability
beta  = 0.03         # Mortality
R1    = 5.           # Contacts per day
R2    = 1./14.       # Inverse recovery time
R3    = 1./14.       # Inverse time until death

I0    = 1.           # Initial infectious population
```

We set up the simulation frame and create a field for our state vector $\vec{Y}$ and initialize it with the initial conditions. The task of the simulation frame is to simulate the evolution of said state vector.

$$\vec{Y} = \begin{pmatrix} S \\ I \\ R \\ D \end{pmatrix}$$

[2]:
```
Y0 = [
    N-I0,  # Susceptible
    I0,    # Infectious
    0.,    # Recovered
    0.     # Deceased
]
```

[3]:
```
from simframe import Frame
```

[4]:
```
sim = Frame(description="SIRD Model")
```

[5]:
```
sim.addfield("Y", Y0, description="State Vector")
```

We create a group in which we store the model parameters.

[6]:
```
sim.addgroup("pars", description="Model Parameters")
sim.pars.addfield("alpha", alpha, description="Transmission probability")
sim.pars.addfield("beta", beta, description="Recovery probability")
sim.pars.addfield("R1", R1, description="Contact rate")
sim.pars.addfield("R2", R2, description="Inverse recovery time")
sim.pars.addfield("R3", R3, description="Inverse time until death")
sim.pars.addfield("N", N, description="Total population size")
```

Additionally, we add fields for the basic reproduction number and for the reproduction number for later analysis.

[7]:
```
sim.pars.addfield("Rt", 0., description="Time-dependent reproduction number")
sim.pars.addfield("R0", 0., description="Basic reproduction number")
```

We then define and add updaters to the reproduction numbers that calculate the numbers from the current state of the simulation frame. The compartments group, that is used in the updater of the time-dependent reproduction number, will be defined later.

[8]:
```
def f_R0(sim):
    alpha, beta = sim.pars.alpha, sim.pars.beta
    R1, R2, R3 = sim.pars.R1, sim.pars.R2, sim.pars.R3
    return alpha*R1/(beta*R2+(1-beta)*R3)
```

[9]:
```
def f_Rt(sim):
    return sim.pars.R0*sim.comp.S/sim.pars.N
```

[10]:
```
sim.pars.R0.updater = f_R0
sim.pars.Rt.updater = f_Rt
```

Additionally we add an updater for the total population size, which is simply the sum of the state vector. In our model the population size will be constant, size we are not considering births.

[11]:
```
def f_N(sim):
    return sim.Y.sum()
```

[12]:
```
sim.pars.N.updater = f_N
```

Now we tell the simulation frame that it has to update the reproduction numbers and the population size in the parameters group.

[13]:
```
sim.pars.updater = ["R0", "Rt", "N"]
```

For convenience we create a group for the compartments and simply copy the elements of the state vector into them in the systole of the compartment updater.

[14]:
```
sim.addgroup("comp", description="Model Compartments")
sim.comp.addfield("S", sim.Y[0], description="Susceptible")
sim.comp.addfield("I", sim.Y[1], description="Infectious")
sim.comp.addfield("R", sim.Y[2], description="Recovered")
sim.comp.addfield("D", sim.Y[3], description="Deceased")
```

[15]:
```
def f_comp_systole(sim):
    sim.comp.S[:] = sim.Y[0]
    sim.comp.I[:] = sim.Y[1]
    sim.comp.R[:] = sim.Y[2]
    sim.comp.D[:] = sim.Y[3]
```

[16]:
```
sim.comp.updater.systole = f_comp_systole
```

Finally, we have to tell the main simulation frame to update the compartments and parameters groups.

[17]:
```
sim.updater = ["comp", "pars"]
```

Now we have to write a function that returns the derivative of our state vector.

[18]:
```
def f_dYdt(sim, x, Y):

    S, I, R, D = Y
    alpha, beta, R1, R2, R3, N = sim.pars.alpha, sim.pars.beta, sim.pars.R1, sim.pars.R2,
↪ sim.pars.R3, sim.pars.N

    dY = np.empty_like(sim.Y)

    dY[0] = -alpha*R1*S*I/N
    dY[2] = (1.-beta)*R2*I
```

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```
    dY[3] = beta*R3*I
    dY[1] = -(dY[0]+dY[2]+dY[3])

    return dY
```

And assign it to the differentiator of the field.

[19]:
```
sim.Y.differentiator = f_dYdt
```

In the next step we have to set up the integration variable.

[20]:
```
sim.addintegrationvariable("t", 0., description="Time [days]")
```

We want to run the simulation for 1 year and have an output every day.

[21]:
```
import numpy as np
```

[22]:
```
sim.t.snapshots = np.arange(1., 366., 1.)
```

We limit the time step, such that no compartment can fall below 0 or can be larger than the population size. We add an CFL factor as safety margin.

[23]:
```
def f_dt(sim):

    cfl = 0.3

    dY = sim.Y.derivative()
    bounds = (0., sim.pars.N)

    rneg = (sim.Y-bounds[0])/dY
    rpos = (bounds[1]-sim.Y)/dY

    dtneg = np.where(dY<0., cfl*np.abs(rneg), 1.e100).min()
    dtpos = np.where(dY>0., cfl*np.abs(rpos), 1.e100).min()

    dt = np.minimum(dtneg, dtpos)

    return dt
```

[24]:
```
sim.t.updater = f_dt
```

We add a single integration instruction and integrate the state vector with the classical 4th order Runge-Kutta scheme.

[25]:
```
from simframe import Integrator
from simframe import Instruction
from simframe import schemes
```

[26]:
```
sim.integrator = Integrator(sim.t)
```

[27]:
```
sim.integrator.instructions = [
    Instruction(schemes.expl_4_runge_kutta, sim.Y)
]
```

We do not want to write output files. Instead we save the data in the simulation frame using the namespace writer. We set the verbosity to zero, because we do not want the writer to print every output on screen.

[28]:
```
from simframe import writers
```

[29]:
```
sim.writer = writers.namespacewriter
sim.writer.verbosity = 0
```

Before we start the simulation we have to update the frame to calculate the initial values of the reproduction numbers.

[30]:
```
sim.update()
```

The complete structure of the model looks like this

[31]:
```
sim.toc
```

```
Frame (SIRD Model)
    - comp: Group (Model Compartments)
        - D: Field (Deceased)
        - I: Field (Infectious)
        - R: Field (Recovered)
        - S: Field (Susceptible)
    - pars: Group (Model Parameters)
        - alpha: Field (Transmission probability)
        - beta: Field (Recovery probability)
        - N: Field (Total population size)
        - R0: Field (Basic reproduction number)
        - R1: Field (Contact rate)
        - R2: Field (Inverse recovery time)
        - R3: Field (Inverse time until death)
        - Rt: Field (Time-dependent reproduction number)
    - t: IntVar (Time [days]), Integration variable
    - Y: Field (State Vector)
```

The simulation is now ready to run.

[32]:
```
sim.run()
```

```
Execution time: 0:00:02
```

We can now read the data and plot the results.

[33]:
```
data = sim.writer.read.all()
```

[34]:
```
from matplotlib import pyplot as plt
```

[35]:
```
def plot_model(data):
    fig, ax = plt.subplots(dpi=150.)
    for c in data.comp.__dict__:
        ax.plot(data.t, data.comp.__dict__[c]/data.pars.N, label=c)
    ax.plot(0., 0., ":", c="black", label="$R_t$")
    ax.legend(loc="upper right")
    ax.set_xlim(data.t[0], data.t[-1])
    ax.set_ylim(-0.1, 1.1)
```

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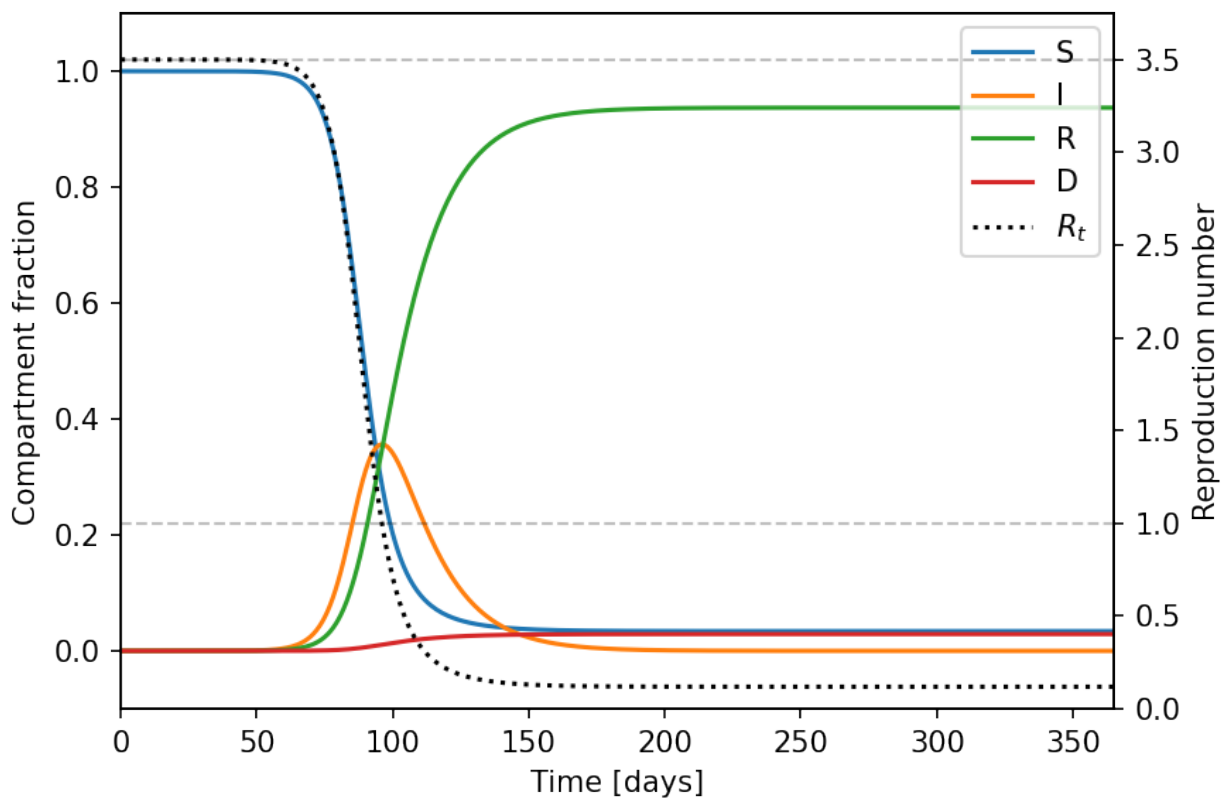
```
    ax.set_xlabel("Time [days]")
    ax.set_ylabel("Compartment fraction")
    axr = ax.twinx()
    axr.plot(data.t, data.pars.Rt, ":", c="black")
    axr.axhline(1., ls="--", lw=1, c="black", alpha=0.25, zorder=-1)
    axr.axhline(data.pars.R0[0], ls="--", lw=1, c="black", alpha=0.25, zorder=-1)
    axr.set_ylabel("Reproduction number")
    axr.set_ylim(0., sim.pars.R0[0]+0.25)
    fig.tight_layout()
    return fig, ax
```

[36]:
```
fig, ax = plot_model(data)
```



In addition to the compartments we plot the reproduction number and horizontal lines for values of reproduction numbers for 1 and the base reproduction number R_0. If the reproduction number is smaller than 1, the population of the infectious compartment decreases, which can be easily seen in the plot.

We can also print the final state on screen

[37]:
```
def print_state(sim):
    for c in sim.comp.__dict__:
        if c.startswith("_"): continue
        print("{:}: {:5.1f} %".format(c, sim.comp.__dict__[c]/sim.pars.N*100.))
    print("Rt: {:5.2f}".format(sim.pars.Rt))
```

[38]:
```
print_state(sim)
```

```
S:   3.4 %
I:   0.0 %
R:  93.7 %
D:   2.9 %
Rt:  0.12
```

At the end of the simulation about 2.9 % of the total population is deceased. This is very close to β as it should be, since almost the entire population got infected by the end of the simulation.

At the peak of the infection wave about 100 days after patient zero about 36 % of the population is infectious.

[39]:
```
print("I_max: {:4.1f} %".format((data.comp.I/data.pars.N).max()*100.))
```

```
I_max: 35.6 %
```

So far our model parameters have been constant with time. But let us assume the following situation.

About 6 % of the people infected with our fictitious disease need to be treated in an intensive care unit (ICU). That means that at the peak of the wave the ICUs needed a capacity of about 2 % of the total population. Typical OECD countries have about 10 ICU beds per 100 000 population. In our scenario the health care system would be completely overwhelmed by the critial patients potentially increasing the chance of dying because of insufficiant medical care.

We are going to run the simulation again assuming that 6 % of the infectious require intensive care and further assuming that those patients without a needed ICU bed have a 30 times higher chance of dying. We can achieve this by increasing our β parameter accordingly and calculate an effective β parameter.

$\beta = \beta_0 \left[1 + \frac{I_{\mathrm{w/o}}}{I}(f-1)\right]$

with β_0 being the unmodified mortality, $I_{\mathrm{w/o}}$ the number of infected without an ICU bed that need one, and f a factor that increases the mortality for the latter.

[40]:
```
def f_beta_effective(sim):

    N = sim.pars.N
    I = sim.comp.I

    # Maximum number of ICU beds
    max_icu = 10./100_000. * N
    # Infected requiring ICU bed
    icu_req = 0.06*I
    # Patients without ICU bed
    I_wo = np.maximum(icu_req - max_icu, 0.)
    # Increase in mortality
    f = 30.

    return beta*(1+I_wo/I*(f-1))
```

[41]:
```
sim.pars.beta.updater = f_beta_effective
```

We then have to add the β parameters to the update order of the parameters group.

[42]:
```
sim.pars.updater = sim.pars.updateorder + ["beta"]
```

We can now reset the simulation and run it again.

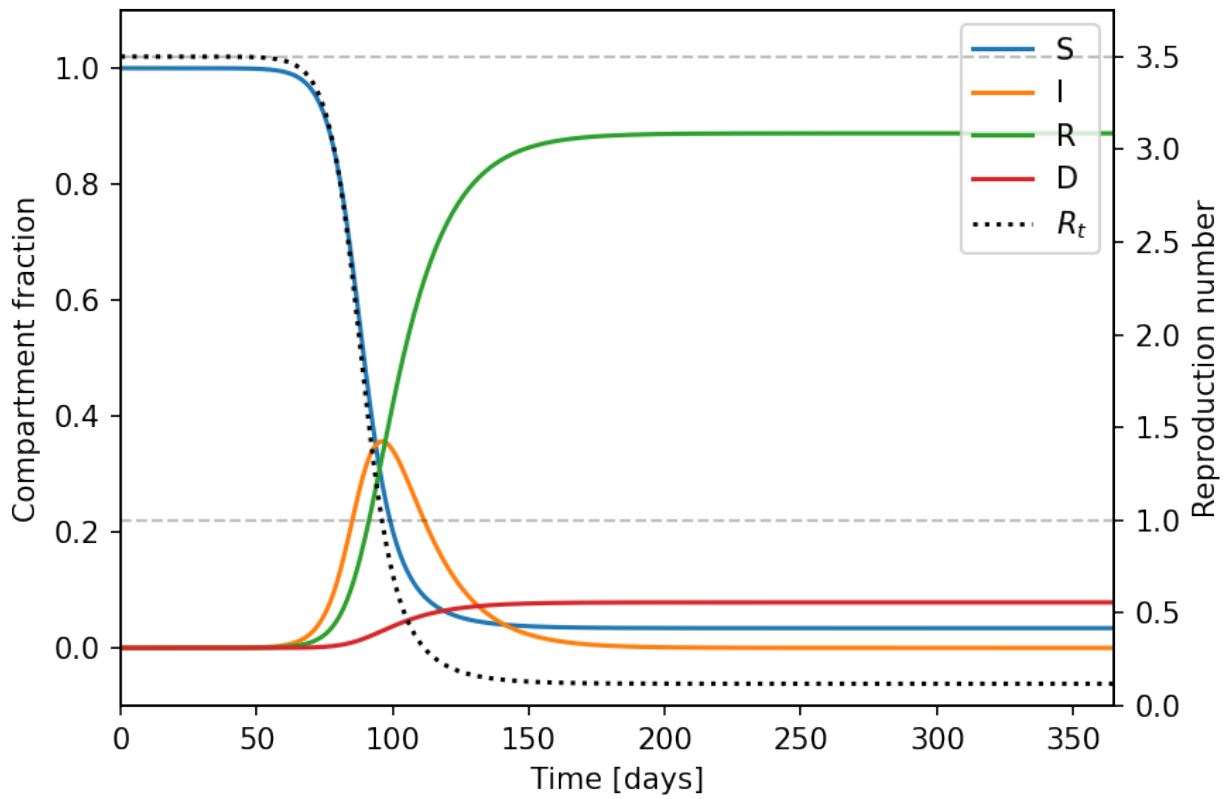
[43]:
```
sim.Y = Y0
sim.t = 0.
sim.update()
sim.writer.reset()
```

[44]:
```
sim.run()
```

```
Execution time: 0:00:01
```

[45]:
```
data_icu = sim.writer.read.all()
```

[46]:
```
fig, ax = plot_model(data_icu)
```



[47]:
```
print_state(sim)
```

```
S:   3.4 %
I:   0.0 %
R:  88.8 %
D:   7.8 %
Rt:  0.12
```

As can be seen the fraction of deceased is with almost 8 % more than twice as large as before, which accounts in our case to almost 500 000 additional casualties.

[48]:
```
print("Additional casualties: {:d}".format(int(N*(0.078-0.029))))
```

```
Additional casualties: 490000
```

We can now further assume that some fictitious government implements some kind of contact restrictions as soon as the the ICU occupancy reaches a certain threshold. We can implement this in our model by reducing our R_1 parameter – the contact rate – accordingly. We assume that contact restrictions are implemented as soon as the ICU occupancy reaches $90\,\%$, which reduces the contact rate to $50\,\%$ of the initial value, and are lifted again as soon as the ICU occupation drops below $50\,\%$ again. We have therefore two thresholds and we need to know if restrictions are in place when crossing them. We are going to introduce a boolean parameter that stores if contact restrictions are in place or not.

[49]:
```
sim.pars.addfield("contact_restrictions", False, description="Contact Restrictions")
```

[50]:
```
def f_R1(sim):

    N = sim.pars.N
    I = sim.comp.I
    restr = sim.pars.contact_restrictions

    # Maximum number ICU beds
    max_icu = 10./100_000. * N
    # Infected requiring ICU bed
    icu_req = 0.06*I
    # ICU occupation
    icu_occup = icu_req/max_icu

    # Lower and upper thresholds
    threshold = (0.5, 0.9)

    # Check if the restriction status changes
    # If restrictions are in place and occupancy falls below threshold or
    # if restrictions are not in place and occupancy goes above threshold
    # we flip the contact restriction state
    if (restr and icu_occup<threshold[0]) or (not restr and icu_occup>threshold[1]):
        sim.pars.contact_restrictions = not restr

    # If we are restricted return lower contact rate
    if restr:
        return 0.5*R1

    # If we are not restriction return unperturbed contact rate
    return R1
```

[51]:
```
sim.pars.R1.updater = f_R1
```

And we have to add the updater to the list. The updater has to be inserted before the reproduction numbers, since they depend on R_1.

[52]:
```
sim.pars.updater = ["R1"] + sim.pars.updateorder
```

We can reset the simulation and run it again.

[53]:
```
sim.Y = Y0
sim.t = 0.
```

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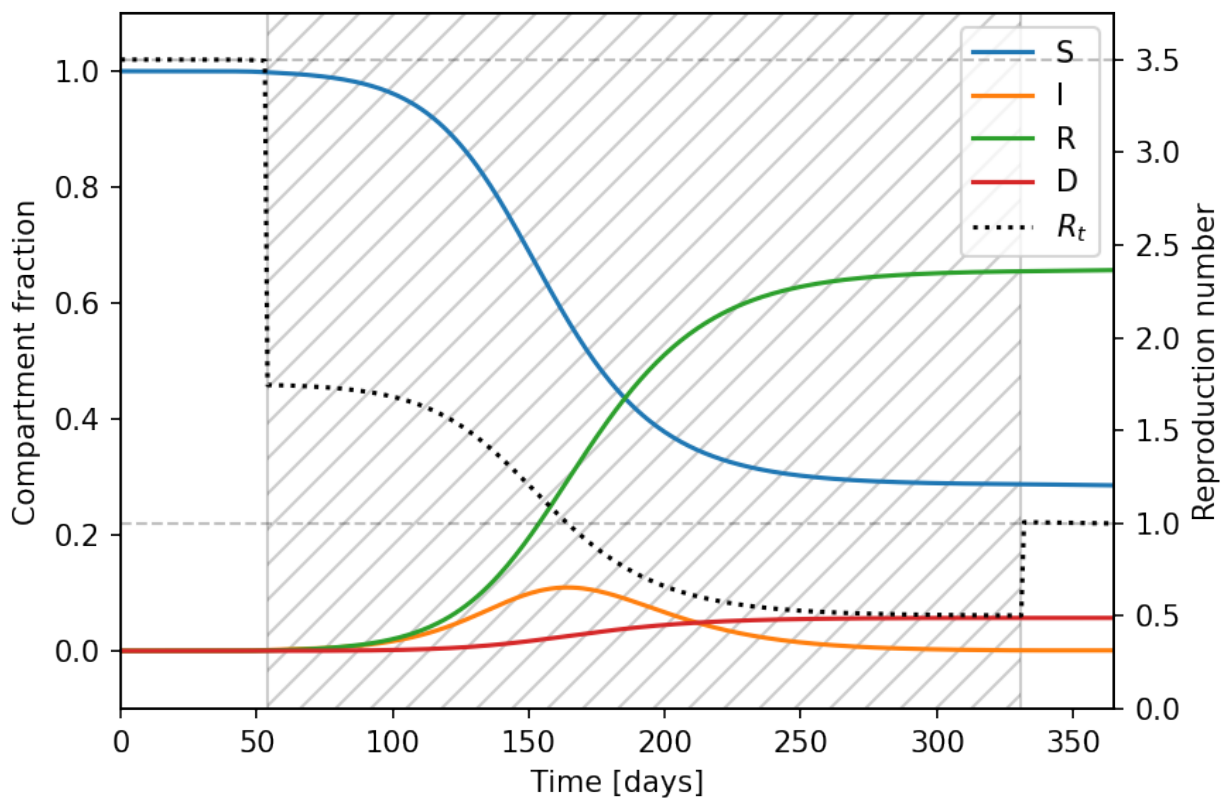
```
sim.update()
sim.writer.reset()
```

[54]:
```
sim.run()
```

```
Execution time: 0:00:01
```

[55]:
```
data_restr = sim.writer.read.all()
```

[56]:
```
fig, ax = plot_model(data_restr)
i0 = data_restr.pars.contact_restrictions.argmax()
i1 = len(data.t)-data_restr.pars.contact_restrictions[::-1].argmax()-1
ax.axvspan(data_restr.t[i0], data_restr.t[i1], edgecolor="#000000", facecolor="None",␣
↪hatch="//", alpha=0.2)
plt.show()
```



[57]:
```
print_state(sim)
```

```
S:  28.6 %
I:   0.1 %
R:  65.7 %
D:   5.7 %
Rt:  1.00
```

It is immeadiately visible that the peak of the infectious compartment is at only 11 % as opposed to the 36 % without restrictions.

[58]:
```
print("I_max: {:4.1f} %".format((data_restr.comp.I/data_restr.pars.N).max()*100.))
```

```
I_max: 10.9 %
```

The contact restrictions – the shaded region – are in place for about 330 days.

[59]:
```
i0 = data_restr.pars.contact_restrictions.argmax()
i1 = len(data_restr.pars.contact_restrictions) - data_restr.pars.contact_restrictions[::-
↪1].argmax() - 1
print("Contact restrictions in place for {:d} days.".format(int(data_restr.t[i1]-data_
↪restr.t[0])))
```

```
Contact restrictions in place for 331 days.
```

At the end of the simulation the fraction of deceased is at about 6 %. Compared to our simulation without restrictions about 210 000 lives were saved.

[60]:
```
print("Lives saved by contact restrictions: {:d}".format(int(N*(0.078-0.057))))
```

```
Lives saved by contact restrictions: 209999
```

After the contact restrictions have been lifted, the reproduction number is stable at one, meaning the spread of the disease is contained.

This model could also be used in the opposite direction. If the structured of the compartmental model is known, the model could be fitted to the data to get the disease parameters.

9.2 SECIR Model

As a second example we want to discuss the SECIR model described by Khailaie et al. (2020) to model the outbreak of SARS-CoV-2.

The model has eight compartments: Susceptible, Exposed, Carrier, Infected, Recovered, Hospitalized, Intensive Care Unit, and Dead. Compartments C and I are infectious and can infect individuals from compartment S. The differential equations governing the system are given by

$$\frac{\mathrm{d}}{\mathrm{d}t}S = -R_1\frac{C+\beta I}{N}S$$

$$\frac{\mathrm{d}}{\mathrm{d}t}E = R_1\frac{C+\beta I}{N}S - R_2E$$

$$\frac{\mathrm{d}}{\mathrm{d}t}C = R_2E - \left[(1-\alpha)\,R_3 + \alpha R_9\right]C$$

$$\frac{\mathrm{d}}{\mathrm{d}t}I = (1-\alpha)\,R_3C - \left[(1-\rho)\,R_4 + \rho R_6\right]I$$

$$\frac{\mathrm{d}}{\mathrm{d}t}H = \rho R_6I - \left[(1-\vartheta)\,R_5 + \vartheta R_7\right]H$$

$$\frac{\mathrm{d}}{\mathrm{d}t}U = \vartheta R_7H - \left[(1-\delta)\,R_8 + \delta d\right]U$$

$$\frac{\mathrm{d}}{\mathrm{d}t}R = \alpha R_9C + (1-\rho)\,R_4I + (1-\vartheta)\,R_5H + (1-\delta)\,R_8U$$

$$\frac{\mathrm{d}}{\mathrm{d}t}D = \delta dU$$

The system can be graphically represented with this chart from Khailaie et al. (2020):

R_1 is the product of median contact frequency and the transmission probability per contact of a susceptible (S) and an infectious (C or I) person. $\beta < 1$ represents the combined risk attenuation factor of infection from symptomatic patients and patients that have not self-isolated effectively, yet. $\frac{1}{R_2}$ is the median time until an exposed person becomes infectious. $\frac{1}{R_2} + \frac{1}{R_3}$ is the incubation period. α is the fraction of asymptomatic cases.

ρ is the fraction of symptomatic cases that require to be hopitalized. $\frac{1}{R_4}$ is the median time until a symptomatic case recovers. $\frac{1}{R_6}$ is the median time until a symptomatic case gets admitted to the hospital. ϑ is the fraction of hospitalized patients that require intesive care. And δ is the fraction of intensive care patients that die. $\frac{1}{R_5}$ and $\frac{1}{R_8}$ are the median times until hospitalized patients and intensive care patients recover. $\frac{1}{R_9}$ is the median time an asymptomatic case remains infectious. And $\frac{1}{d}$ is the median time until intensive care patients die.

In this model the basic reproduction number is given by

$R_0 = R_1 \frac{R_4(1-\rho)+R_3\beta(1-\alpha)+R_6\rho}{[R_3(1-\alpha)+R_9\alpha][R_4(1-\rho)+R_6\rho]}$.

The time-dependent reproduction number is given by

$R_t = R_0 \frac{S}{N}$

These parameters can all vary with time, country, culture, and healthcare system. Khailaie et al. (2020) used parameters from a fit to early data from Italy.

We are going to use the following values in this example

- $R_1 = 0.587\,\text{days}$
- $\frac{1}{R_2} = 5.2\,\text{days} - \frac{1}{R_3}$ (Incubation period is $5.2\,\text{days}$)
- $R_3 = \frac{1}{4.2\,\text{days}}$
- $R_4 = \frac{1}{14\,\text{days}}$
- $R_5 = \frac{1}{16\,\text{days}}$
- $R_6 = \frac{1}{2.5\,\text{days}}$
- $R_7 = \frac{1}{3.5\,\text{days}}$
- $R_8 = \frac{1}{16\,\text{days}}$
- $\frac{1}{R_9} = \frac{1}{R_3} + \frac{1}{2R_4}$
- $d = \frac{1}{6.92\,\text{days}}$
- $\alpha = 0.01$
- $\beta = 0.05$
- $\delta = 0.15$
- $\vartheta = 0.15$
- $\delta = 0.35$

As before we are going to set up the model.

[61]:
```
sim = Frame(description="Khailaie et al. (2020)")
```

[62]:
```
sim.addgroup("pars", description="Model parameters")
sim.pars.addfield("N", 0., description="Population size")
sim.pars.addfield("R0", 0., description="Basic reproduction number")
sim.pars.addfield("Rt", 0., description="Time-dependent reproduction number")
sim.pars.addfield("R1", 0., description="S -> E")
sim.pars.addfield("R2", 0., description="E -> C")
sim.pars.addfield("R3", 0., description="C -> I")
sim.pars.addfield("R4", 0., description="I -> R")
sim.pars.addfield("R5", 0., description="H -> R")
```

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```
sim.pars.addfield("R6", 0., description="I -> H")
sim.pars.addfield("R7", 0., description="H -> U")
sim.pars.addfield("R8", 0., description="U -> R")
sim.pars.addfield("R9", 0., description="C -> R")
sim.pars.addfield("d", 0., description="U -> D")
sim.pars.addfield("alpha", 0., description="Probability of asymptotic case")
sim.pars.addfield("beta", 0., description="Infection attenuation")
sim.pars.addfield("delta", 0., description="Mortality")
sim.pars.addfield("theta", 0., description="ICU probability")
sim.pars.addfield("rho", 0., description="Hospitalization probability")
```

[63]:
```
sim.pars.N = 10_000_000.
sim.pars.R1 = 0.587
sim.pars.R3 = 1./4.2
sim.pars.R4 = 1./14.
sim.pars.R5 = 1./16.
sim.pars.R6 = 1./2.5
sim.pars.R7 = 1./3.5
sim.pars.R8 = 1./16.
sim.pars.d = 1./6.92
sim.pars.alpha = 0.01
sim.pars.beta = 0.05
sim.pars.delta = 0.15
sim.pars.theta = 0.15
sim.pars.rho = 0.35
```

We define updater for some of the parameters.

[64]:
```
def f_N(sim):
    return sim.Y.sum()
```

[65]:
```
def f_R0(sim):
    R1, R3, R4, R6, R9 = sim.pars.R1, sim.pars.R3, sim.pars.R4, sim.pars.R6, sim.pars.R9
    alpha, beta, rho = sim.pars.alpha, sim.pars.beta, sim.pars.rho
    return R1 * (R4*(1.-rho) + R3*beta*(1.-alpha) + R6*rho) / (R3*(1.-alpha) + R9*alpha)␣
↪/ (R4*(1.-rho) + R6*rho)
```

[66]:
```
def f_Rt(sim):
    return sim.pars.R0*sim.comp.S/sim.pars.N
```

[67]:
```
def f_R2(sim):
    inv = 5.2 - 1./sim.pars.R3
    return 1./inv
```

[68]:
```
def f_R9(sim):
    inv = 1./sim.pars.R3 + 0.5/sim.pars.R4
    return 1./inv
```

[69]:
```
sim.pars.N.updater = f_N
sim.pars.R0.updater = f_R0
```

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```
sim.pars.Rt.updater = f_Rt
sim.pars.R2.updater = f_R2
sim.pars.R9.updater = f_R9
```

[70]:
```
sim.pars.updater = ["N", "R2", "R9", "R0", "Rt"]
```

Again we store the comnpartments in the state vecotr $\vec{Y}$.

[71]:
```
Y = [sim.pars.N[0]-1, 0., 1., 0., 0., 0., 0., 0.]
```

[72]:
```
sim.addfield("Y", Y, description="State vector")
```

[73]:
```
sim.addgroup("comp", description="Compartments")
sim.comp.addfield("S", 0., description="Susceptible")
sim.comp.addfield("E", 0., description="Exposed")
sim.comp.addfield("C", 0., description="Carrier")
sim.comp.addfield("I", 0., description="Infected")
sim.comp.addfield("H", 0., description="Hospitalized")
sim.comp.addfield("U", 0., description="Intensive Care Unit")
sim.comp.addfield("R", 0., description="Recovered")
sim.comp.addfield("D", 0., description="Dead")
```

And just copy their values into the compartments group in the systole.

[74]:
```
def f_comp_systole(sim):
    sim.comp.S = sim.Y[0]
    sim.comp.E = sim.Y[1]
    sim.comp.C = sim.Y[2]
    sim.comp.I = sim.Y[3]
    sim.comp.H = sim.Y[4]
    sim.comp.U = sim.Y[5]
    sim.comp.R = sim.Y[6]
    sim.comp.D = sim.Y[7]
```

[75]:
```
sim.comp.updater.systole = f_comp_systole
```

[76]:
```
sim.updater = ["comp", "pars"]
```

The function with the differential equations.

[77]:
```
def f_dYdt(sim, x, Y):

    S, E, C, I, H, U, R, D = Y
    alpha, beta, delta, theta, rho = sim.pars.alpha, sim.pars.beta, sim.pars.delta, sim.
↪pars.theta, sim.pars.rho
    N, d = sim.pars.N, sim.pars.d
    R1, R2, R3, R4, R5, R6, R7, R8, R9 = sim.pars.R1, sim.pars.R2, sim.pars.R3, sim.pars.
↪R4, sim.pars.R5, sim.pars.R6, sim.pars.R7, sim.pars.R8, sim.pars.R9

    dY = np.zeros_like(Y)
```

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```
    dY[0] = -R1*(C+beta*I)*S/N
    dY[1] = -dY[0] - R2*E
    dY[2] = R2*E - ((1.-alpha)*R3 + alpha*R9)*C
    dY[3] = (1.-alpha)*R3*C - ((1.-rho)*R4+rho*R6)*I
    dY[4] = rho*R6*I - ((1.-theta)*R5+theta*R7)*H
    dY[5] = theta*R7*H - ((1.-delta)*R8+delta*d)*U
    dY[6] = alpha*R9*C + (1.-rho)*R4*I + (1.-theta)*R5*H + (1.-delta)*R8*U
    dY[7] = -dY.sum()  # Since the total population size is constant, the last␣
↪comaprtment is not independent

    return dY
```

[78]:
```
sim.Y.differentiator = f_dYdt
```

And the integration variable. We are going to simulate the model for 180 days.

[79]:
```
sim.addintegrationvariable("t", 0., description="Time [days]")
```

[80]:
```
sim.t.snapshots = np.arange(1., 181., 1.)
```

We are not going to define a custom function for the time step, that ensures that the compartments are always inbound. Instead we are using an adaptive integration scheme. Therefore the time step updater needs to return the suggested time step.

[81]:
```
def f_dt(sim):
    return sim.t.suggested
```

[82]:
```
sim.t.updater = f_dt
```

And we initialize it with a value of 1 day.

[83]:
```
sim.t.suggest(1.)
```

Then we define the integrator with a single integration instruction.

[84]:
```
sim.integrator = Integrator(sim.t)
```

[85]:
```
sim.integrator.instructions = [
    Instruction(schemes.expl_5_cash_karp_adptv, sim.Y)
]
```

We are using the namespace writer and turn off the verbosity.

[86]:
```
sim.writer = writers.namespacewriter()
sim.writer.verbosity = 0
```

The model is now complete.

[87]:
```
sim.toc
```

```
Frame (Khailaie et al. (2020))
    - comp: Group (Compartments)
```

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```
        - C: Field (Carrier)
        - D: Field (Dead)
        - E: Field (Exposed)
        - H: Field (Hospitalized)
        - I: Field (Infected)
        - R: Field (Recovered)
        - S: Field (Susceptible)
        - U: Field (Intensive Care Unit)
    - pars: Group (Model parameters)
        - alpha: Field (Probability of asymptotic case)
        - beta: Field (Infection attenuation)
        - d: Field (U -> D)
        - delta: Field (Mortality)
        - N: Field (Population size)
        - R0: Field (Basic reproduction number)
        - R1: Field (S -> E)
        - R2: Field (E -> C)
        - R3: Field (C -> I)
        - R4: Field (I -> R)
        - R5: Field (H -> R)
        - R6: Field (I -> H)
        - R7: Field (H -> U)
        - R8: Field (U -> R)
        - R9: Field (C -> R)
        - rho: Field (Hospitalization probability)
        - Rt: Field (Time-dependent reproduction number)
        - theta: Field (ICU probability)
    - t: IntVar (Time [days]), Integration variable
    - Y: Field (State vector)
```

Before we can run the simulation we have to update the simulation frame.

[88]:
```
sim.update()
```

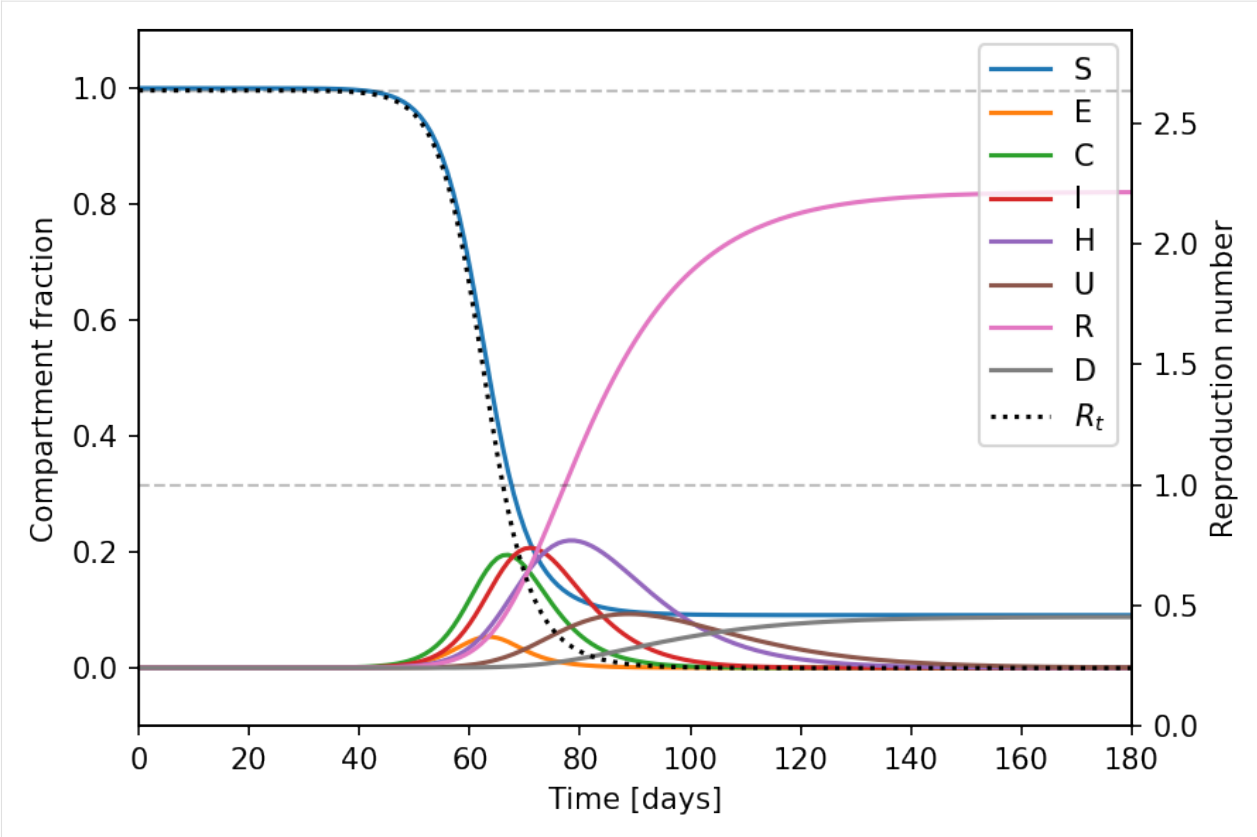
[89]:
```
sim.run()
```

```
Execution time: 0:00:01
```

After the simulation we can plot the results.

[90]:
```
data = sim.writer.read.all()
```

[91]:
```
fig, ax = plot_model(data)
```



[92]:
```
print_state(sim)
```

```
S:   9.1 %
E:   0.0 %
C:   0.0 %
I:   0.0 %
H:   0.0 %
U:   0.1 %
R:  82.1 %
D:   8.8 %
Rt:  0.24
```

At the end of this simulation about 9 % of the population died.

[93]:
```
print("I_max: {:4.1f} %".format((data.comp.U/data.pars.N).max()*100.))
```

```
I_max:  9.3 %
```

At the peak of the infection wave. At the peak of the wave about 9 % of the population would require intensive care overwhelming any healthcare system in the world.

Please note that there are more complex models and updated parameters available by now.

CHAPTER

TEN

APPENDIX A: CITATION

If you use `Simframe`, please remember to cite Stammler & Birnstiel (2022).

```
@article{simframe,
  doi = {10.21105/joss.03882},
  url = {https://doi.org/10.21105/joss.03882},
  year = {2022},
  publisher = {The Open Journal},
  volume = {7},
  number = {69},
  pages = {3882},
  author = {Sebastian M. Stammler and Tilman Birnstiel},
  title = {Simframe: A Python Framework for Scientific Simulations},
  journal = {Journal of Open Source Software}
}
```

CHAPTER

ELEVEN

APPENDIX B: CONTRIBUTING/BUGS/FEATURES

Please have a look at the Contribution Guidelines.

11.1 Contributing to `simframe`

To contribute code please open a new pull request and describe the changes to the software your pull request introduces.

Please note, that we want to achieve a **code coverage of 100%**. Any addition to the software must therefore also come with unit tests. Additional features must also be described in the documentation.

11.2 Bug Report

If you encountered a bug in `simframe`, please open a new bug report issue and describe the bug, the expected behavior, and steps how to reproduce the bug.

11.3 Feature Request

If you have an idea of a new feature, that is missing in `simframe`, or if you want to suggest an improvement, please open a new feature request issue.

CHAPTER

TWELVE

MODULE REFERENCE

12.1 simframe.frame Package

This package contains the core infrastructure of `simframe`.

12.1.1 Classes

AbstractGroup()	This is an abstract class that serves as template for other classes.
Field(owner, value[, updater, ...])	Class for storing simulation quantities.
Frame([integrator, writer, updater, ...])	This is the parent object of type `Group` that contains all other objects.
Group(owner[, updater, description])	Class for grouping data.
Heartbeat([updater, systole, diastole])	This class controls an update including `systole` and `diastole`.
IntVar(owner[, value, snapshots, updater, ...])	Cclass for integration variables that behaves as `Field` but has additional functionality with respect to stepsize management for integration.
Updater([func])	Class that manages how a `Group` or `Field` is updated.

AbstractGroup

class `simframe.frame.`**`AbstractGroup`**

Bases: `object`

This is an abstract class that serves as template for other classes.

`AbstractGroup` has a descriptive string, an owner and an updater. The owner is the parent `Frame` object and is hidden. The updater is of type `Heartbeat`.

`AbstractGroup` has an `update` method that is calling `systole`, `updater`, and `diastole` of the `Heartbeat` object, which manages the update of `AbstractGroup`.

`AbstractGroup` should not be instanciated directly.

Attributes

description

Description of the instance.

updater

`Heatbeat` object with instructions for updating the instance.

Methods

update(*args, **kwargs)	Function to update the object.

Attributes Summary

description	Description of the instance.
updater	`Heatbeat` object with instructions for updating the instance.

Methods Summary

update(*args, **kwargs)	Function to update the object.

Attributes Documentation

description

Description of the instance.

updater

`Heatbeat` object with instructions for updating the instance.

Methods Documentation

update(**args*, ***kwargs*)

Function to update the object. Ths functions calls the heartbeat instance of the object.

Parameters

- **args** (*additional positional arguments*) –
- **kwargs** (*additional keyword arguments*) –

Notes

Positional arguments and keyword arguments are only passed to the `updater`, NOT to `systole` and `diastole`.

Field

class simframe.frame.**Field**(*owner*, *value*, *updater=None*, *differentiator=None*, *jacobinator=None*, *description=''*, *constant=False*, *save=True*, *copy=False*)

Bases: `ndarray`, *AbstractGroup*

Class for storing simulation quantities.

In addition to `Group`, `Field` can have an `differentiator` for calculating its derivative and/or an `jacobinator` for calculating its Jacobian. The function that is calculating the derivative needs the parent `Frame` object as first, the integration variable of type `IntVar` as second, and the `Field` itself as third positional argument

`Field` behaves like `numpy.ndarray` and can perform the same numerical operations.

Notes

When `Field.update()` is called `Field` will be updated according return value of the `updater` of the `Heartbeat` object assigned to the `Field`. The function that is updating `Field` needs the parent `Frame` object as first positional argument.

Attributes

`T`
The transposed array.

`base`
Base object if memory is from some other object.

`buffer`
Temporary buffer that stores the new value of `Field` after successful integration.

`constant`
If True, `Field` is immutable.

`ctypes`
An object to simplify the interaction of the array with the ctypes module.

`data`
Python buffer object pointing to the start of the array's data.

`description`
Description of the instance.

`differentiator`
`Heartbeat` object with instructions for calculating the derivative of `Field`

`dtype`
Data-type of the array's elements.

`flags`
Information about the memory layout of the array.

`flat`
A 1-D iterator over the array.

`imag`
The imaginary part of the array.

`itemsize`
Length of one array element in bytes.

`jacobinator`
`Heartbeat` object with instructions for calculating the Jacobian of `Field`

`nbytes`
Total bytes consumed by the elements of the array.

`ndim`
Number of array dimensions.

`real`
The real part of the array.

`save`
If False, `Field` will not be stored in output files.

shape
Tuple of array dimensions.

size
Number of elements in the array.

strides
Tuple of bytes to step in each dimension when traversing an array.

updater
`Heatbeat` object with instructions for updating the instance.

Methods

`all`([axis, out, keepdims, where])	Returns True if all elements evaluate to True.
`any`([axis, out, keepdims, where])	Returns True if any of the elements of *a* evaluate to True.
`argmax`([axis, out])	Return indices of the maximum values along the given axis.
`argmin`([axis, out])	Return indices of the minimum values along the given axis.
`argpartition`(kth[, axis, kind, order])	Returns the indices that would partition this array.
`argsort`([axis, kind, order])	Returns the indices that would sort this array.
`astype`(dtype[, order, casting, subok, copy])	Copy of the array, cast to a specified type.
`byteswap`([inplace])	Swap the bytes of the array elements
`choose`(choices[, out, mode])	Use an index array to construct a new array from a set of choices.
`clip`([min, max, out])	Return an array whose values are limited to `[min, max]`.
`compress`(condition[, axis, out])	Return selected slices of this array along given axis.
`conj`()	Complex-conjugate all elements.
`conjugate`()	Return the complex conjugate, element-wise.
`copy`([order])	Return a copy of the array.
`cumprod`([axis, dtype, out])	Return the cumulative product of the elements along the given axis.
`cumsum`([axis, dtype, out])	Return the cumulative sum of the elements along the given axis.
`derivative`([x, Y])	If `differentiator` or `jacobinator` is set, this returns the derivative of the `Field`.
`diagonal`([offset, axis1, axis2])	Return specified diagonals.
`dot`(b[, out])	Dot product of two arrays.
`dump`(file)	Dump a pickle of the array to the specified file.
`dumps`()	Returns the pickle of the array as a string.
`fill`(value)	Fill the array with a scalar value.
`flatten`([order])	Return a copy of the array collapsed into one dimension.
`getfield`(dtype[, offset])	Returns a field of the given array as a certain type.
`item`(*args)	Copy an element of an array to a standard Python scalar and return it.
`itemset`(*args)	Insert scalar into an array (scalar is cast to array's dtype, if possible)

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Table 1 – continued from previous page

jacobian([x])	If `jacobinator` is set, this returns the Jacobi matrix of the `Field`.
`max`([axis, out, keepdims, initial, where])	Return the maximum along a given axis.
`mean`([axis, dtype, out, keepdims, where])	Returns the average of the array elements along given axis.
`min`([axis, out, keepdims, initial, where])	Return the minimum along a given axis.
`newbyteorder`([new_order])	Return the array with the same data viewed with a different byte order.
`nonzero`()	Return the indices of the elements that are non-zero.
`partition`(kth[, axis, kind, order])	Rearranges the elements in the array in such a way that the value of the element in kth position is in the position it would be in a sorted array.
`prod`([axis, dtype, out, keepdims, initial, ...])	Return the product of the array elements over the given axis
`ptp`([axis, out, keepdims])	Peak to peak (maximum - minimum) value along a given axis.
`put`(indices, values[, mode])	Set `a.flat[n] = values[n]` for all *n* in indices.
`ravel`([order])	Return a flattened array.
`repeat`(repeats[, axis])	Repeat elements of an array.
`reshape`(shape[, order])	Returns an array containing the same data with a new shape.
`resize`(new_shape[, refcheck])	Change shape and size of array in-place.
`round`([decimals, out])	Return *a* with each element rounded to the given number of decimals.
`searchsorted`(v[, side, sorter])	Find indices where elements of v should be inserted in a to maintain order.
`setfield`(val, dtype[, offset])	Put a value into a specified place in a field defined by a data-type.
`setflags`([write, align, uic])	Set array flags WRITEABLE, ALIGNED, (WRITEBACKIFCOPY and UPDATEIFCOPY), respectively.
`sort`([axis, kind, order])	Sort an array in-place.
`squeeze`([axis])	Remove axes of length one from *a*.
`std`([axis, dtype, out, ddof, keepdims, where])	Returns the standard deviation of the array elements along given axis.
`sum`([axis, dtype, out, keepdims, initial, where])	Return the sum of the array elements over the given axis.
`swapaxes`(axis1, axis2)	Return a view of the array with *axis1* and *axis2* interchanged.
`take`(indices[, axis, out, mode])	Return an array formed from the elements of *a* at the given indices.
`tobytes`([order])	Construct Python bytes containing the raw data bytes in the array.
`tofile`(fid[, sep, format])	Write array to a file as text or binary (default).
`tolist`()	Return the array as an `a.ndim`-levels deep nested list of Python scalars.
`tostring`([order])	A compatibility alias for *tobytes*, with exactly the same behavior.
`trace`([offset, axis1, axis2, dtype, out])	Return the sum along diagonals of the array.
`transpose`(*axes)	Returns a view of the array with axes transposed.
update(*args, **kwargs)	Function to update the `Field`.

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Table 1 – continued from previous page

var([axis, dtype, out, ddof, keepdims, where])	Returns the variance of the array elements, along given axis.
view([dtype][, type])	New view of array with the same data.

Attributes Summary

buffer	Temporary buffer that stores the new value of `Field` after successful integration.
constant	If True, `Field` is immutable.
differentiator	`Heartbeat` object with instructions for calculating the derivative of `Field`
jacobinator	`Heartbeat` object with instructions for calculating the Jacobian of `Field`
save	If False, `Field` will not be stored in output files.

Methods Summary

derivative([x, Y])	If `differentiator` or `jacobinator` is set, this returns the derivative of the `Field`.
jacobian([x])	If `jacobinator` is set, this returns the Jacobi matrix of the `Field`.
update(*args, **kwargs)	Function to update the `Field`.

Attributes Documentation

buffer

Temporary buffer that stores the new value of `Field` after successful integration.

constant

If True, `Field` is immutable.

differentiator

`Heartbeat` object with instructions for calculating the derivative of `Field`

jacobinator

`Heartbeat` object with instructions for calculating the Jacobian of `Field`

save

If False, `Field` will not be stored in output files.

Methods Documentation

derivative(*x=None*, *Y=None*, **args*, ***kwargs*)

If `differentiator` or `jacobinator` is set, this returns the derivative of the `Field`.

Parameters

- **x** (`IntVar, optional, default : None`) – Integration variable If None it uses the integration variable of the integrator of the parent Frame
- **Y** (`Field, optional, default : None`) – Derivative of Y with respect to the integration variable. If None it uses the field itself

Returns
deriv

Return type
derivative of the field according the differetiator or jacobinator

Notes

The function that calculates the derivative needs the parent `Frame` as first positional, the integration variable `IntVar` as second positional, and the `Field` itself as third positional argument.

The `differentiator` is not set, it will try to calculate the derivative from the Jacobian. If `jacobinator` is also not set, it will return `False`

jacobian(*x=None*, **args*, ***kwargs*)

If `jacobinator` is set, this returns the Jacobi matrix of the `Field`.

Parameters
x (`IntVar, optional, default : None`) – Integration variable If None it uses the integration variable of the integrator of the parent Frame

Returns

- **jac** (*Jacobi matrix of the field according the differetiator*)
- *The function that calculates the Jacobian needs the parent frame as first positional and the*
- *integration variable as second positional.*

update(**args*, ***kwargs*)

Function to update the `Field`.

Frame

class simframe.frame.**Frame**(*integrator=None*, *writer=None*, *updater=None*, *verbosity=2*, *progressbar=None*, *description=''*)

Bases: `Group`

This is the parent object of type `Group` that contains all other objects.

During integration the `update()` function of the `Frame` object will be called. You have to sub-delegete the updates of your other `Group` and `Field` objects within this function.

`Frame` has additional functionality for writing output files and for integration.

Attributes

description
Description of the instance.

integrator
`Integrator` that controls the simulation.

progressbar
`Progressbar` for displaying current status.

toc
Complete table of contents starting from this object.

updateorder
Update order if updater was set with list of strings.

updater
`Heartbeat` object with update instructions.

verbosity
Verbosity of the `Frame` objects.

writer
`Writer` object for writing output files.

Methods

`addfield`(name, value[, updater, ...])	Function to add a new `Field` to the object.
`addgroup`(name[, updater, description])	Function to add a new `Group` to the object.
`addintegrationvariable`(name, value[, ...])	Function to add a new integration variable `IntVar` to the object.
`memory_usage`([print_output, skip_hidden])	Determine memory usage of a Group
run()	This method starts the simulation.
`update`(*args, **kwargs)	Function to update the object.
writeoutput([i, forceoverwrite, filename])	Writes output to file, if `Writer` is specified.

Attributes Summary

integrator	`Integrator` that controls the simulation.
progressbar	`Progressbar` for displaying current status.
verbosity	Verbosity of the `Frame` objects.
writer	`Writer` object for writing output files.

Methods Summary

run()	This method starts the simulation.
writeoutput([i, forceoverwrite, filename])	Writes output to file, if `Writer` is specified.

Attributes Documentation

integrator

`Integrator` that controls the simulation.

progressbar

`Progressbar` for displaying current status.

verbosity

Verbosity of the `Frame` objects.

writer

`Writer` object for writing output files.

Methods Documentation

run()

This method starts the simulation. An `Integrator` has to be set beforehand.

writeoutput(*i=0*, *forceoverwrite=False*, *filename=''*, ***kwargs*)

Writes output to file, if `Writer` is specified.

Parameters

- **i** (*int, optional, default : 0*) – Number of output
- **forceoverwrite** (*boolean, optional, default : False*) – If True, this overrules the seetings of the Writer and enforces the file to be overwritten.
- **filename** (*string, optional, default = ""*) – if given this will write the output to this file. Otherwise, it uses the standard scheme.
- **kwargs** (*additional keyword arguments*) – Additional options that can be passed to the writer

Group

class simframe.frame.**Group**(*owner*, *updater=None*, *description=''*)

Bases: *AbstractGroup*

Class for grouping data. `Group` is a data frame that has additional functionality for updating its attributes.

Notes

When `Group.update()` is called the instructions of the group's `Heartbeat` object will be performed. The function that is determing the update operation needs the parent `Frame` object as first positional argument.

Attributes

description

Description of the instance.

toc

Complete table of contents starting from this object.

updateorder

Update order if updater was set with list of strings.

updater
Heartbeat object with update instructions.

Methods

addfield(name, value[, updater, ...])	Function to add a new Field to the object.
addgroup(name[, updater, description])	Function to add a new Group to the object.
addintegrationvariable(name, value[, ...])	Function to add a new integration variable IntVar to the object.
memory_usage([print_output, skip_hidden])	Determine memory usage of a Group
update(*args, **kwargs)	Function to update the object.

Attributes Summary

toc	Complete table of contents starting from this object.
updateorder	Update order if updater was set with list of strings.
updater	Heartbeat object with update instructions.

Methods Summary

addfield(name, value[, updater, ...])	Function to add a new Field to the object.
addgroup(name[, updater, description])	Function to add a new Group to the object.
addintegrationvariable(name, value[, ...])	Function to add a new integration variable IntVar to the object.
memory_usage([print_output, skip_hidden])	Determine memory usage of a Group

Attributes Documentation

toc

Complete table of contents starting from this object.

updateorder

Update order if updater was set with list of strings. None otherwise.

updater

Heartbeat object with update instructions.

You can either set a Heartbeat object directly, a callable functions that will be automatically transformed into a Heartbeat object, or a list of attribute names of the Group that will be updated in that order.

Methods Documentation

addfield(*name*, *value*, *updater=None*, *differentiator=None*, *description=''*, *constant=False*, *save=True*, *copy=True*)

Function to add a new `Field` to the object.

Parameters

- **name** (*string*) – Name of the field
- **value** (*number, array, string*) – Initial value of the field. Needs to have already the correct type and shape
- **updater** (Heartbeat, Updater, *callable or None, optional, default : None*) – Updater for field update
- **differentiator** (Heartbeat, Updater, *callable or None, optional, default : None*) – Differentiator if the field has a derivative
- **description** (*string, optional, default : ""*) – Descriptive string for the field
- **constant** (*boolean, optional, default : False*) – True if the field is immutable
- **save** (*boolean, optional, default : True*) – If True field will be stored in output files
- **copy** (*boolean, optional, default : True*) – If True <value> will be copied, not referenced

addgroup(*name*, *updater=None*, *description=''*)

Function to add a new `Group` to the object.

Parameters

- **name** (*string*) – Name of the group
- **updater** (Heartbeat, Updater, *callable or None, optional, default : None*) – Updater for field update
- **description** (*string, optional, default : ""*) – Descriptive string for the group

addintegrationvariable(*name*, *value*, *snapshots=[]*, *updater=None*, *description=''*, *copy=True*)

Function to add a new integration variable `IntVar` to the object.

Parameters

- **name** (*string*) – Name of the field
- **value** (*number, array, string*) – Initial value of the field. Needs to have already the correct type and shape
- **updater** (Heartbeat, Updater, *callable or None, optional, default : None*) – Updater for field update
- **snapshots** (*list, ndarray, optional, default : []*) – List of snapshots at which an output file should be written
- **description** (*string, optional, default : ""*) – Descriptive string for the field
- **copy** (*boolean, optional, default : True*) – If True <value> will be copied, not referenced

memory_usage(*print_output=False*, *skip_hidden=False*)

Determine memory usage of a Group

Will only return the correct data size of Fields and Groups of Fields. Other data types might deviate from the true memory usage.

Parameters

- **print_output** (*bool, optional, default : False*) – if True, print results on screen
- **skip_hidden** (*bool, optional, default : False*) – if True, hidden attributes will be ignored

Returns
total memory usage of group in bytes

Return type
float

Heartbeat

class simframe.frame.**Heartbeat**(*updater=None*, *systole=None*, *diastole=None*)

Bases: `object`

This class controls an update including `systole` and `diastole`.

A full cardiac cycle constists of a systole operation, the actual update and a systole operation. All three are of type `Updater`.

The `beat` function calls `systole`, `updater`, `diastole` in that order and returns the return value of the `updater`. Any positional or keyword arguments are only passed to the `updater`, NOT to `systole` and `diastole`.

Attributes

diastole
`Updater` that is called at the end of the cardiac cycle.

systole
`Updater` that is called in the beginning of cardiac cycle.

updater
`Updater` that is performing the update instruction.

Methods

beat(owner, *args[, Y])	This method executes `systole`, `updater`, and `distole` in that order and returns the return value of the `updater`.

Attributes Summary

diastole	Updater that is called at the end of the cardiac cycle.
systole	Updater that is called in the beginning of cardiac cycle.
updater	Updater that is performing the update instruction.

Methods Summary

beat(owner, *args[, Y])	This method executes systole, updater, and distole in that order and returns the return value of the updater.

Attributes Documentation

diastole

Updater that is called at the end of the cardiac cycle.

systole

Updater that is called in the beginning of cardiac cycle.

updater

Updater that is performing the update instruction.

Methods Documentation

beat(*owner*, **args*, *Y=None*, ***kwargs*)

This method executes systole, updater, and distole in that order and returns the return value of the updater.

Parameters

- **owner** (Frame) – Parent frame object to which updater belongs
- **Y** (Field, *optional, default : None*) – Field that should be updated

Notes

*args and **kwargs are only passed to updater, NOT to systole and diastole

Returns
ret

Return type
Return value of updater.

IntVar

class simframe.frame.**IntVar**(*owner*, *value=0*, *snapshots=[]*, *updater=None*, *description=''*, *save=True*, *copy=False*)

Bases: *Field*

Cclass for integration variables that behaves as `Field` but has additional functionality with respect to stepsize management for integration.

Notes

The `updater` for integration variables is calculating the stepsize. The function associated to the `updater` needs the parent `Frame` object as first positional argument and needs to return the desired stepsize.

`IntVar.update()` does not update the integration variable. Try not to update the integration variable by hand. Let the `Integrator` do it for you.

Attributes

T
The transposed array.

base
Base object if memory is from some other object.

buffer
Temporary buffer that stores the new value of `Field` after successful integration.

constant
If True, `Field` is immutable.

ctypes
An object to simplify the interaction of the array with the ctypes module.

data
Python buffer object pointing to the start of the array's data.

description
Description of the instance.

differentiator
`Heartbeat` object with instructions for calculating the derivative of `Field`

dtype
Data-type of the array's elements.

flags
Information about the memory layout of the array.

flat
A 1-D iterator over the array.

imag
The imaginary part of the array.

itemsize
Length of one array element in bytes.

jacobinator
`Heartbeat` object with instructions for calculating the Jacobian of `Field`

maxstepsize
Maximum possible step size, i.e., to next snapshot.

nbytes
Total bytes consumed by the elements of the array.

ndim
Number of array dimensions.

nextsnapshot
Value of the next snapshot.

prevsnapshot
Value of the previous snapshot.

prevstepsize
Previously taken step size.

real
The real part of the array.

save
If False, `Field` will not be stored in output files.

shape
Tuple of array dimensions.

size
Number of elements in the array.

snapshots
Snapshots at which output should be written.

stepsize
Current stepsize.

strides
Tuple of bytes to step in each dimension when traversing an array.

suggested
Suggested step size.

updater
`Heatbeat` object with instructions for updating the instance.

Methods

`all`([axis, out, keepdims, where])	Returns True if all elements evaluate to True.
`any`([axis, out, keepdims, where])	Returns True if any of the elements of *a* evaluate to True.
`argmax`([axis, out])	Return indices of the maximum values along the given axis.
`argmin`([axis, out])	Return indices of the minimum values along the given axis.
`argpartition`(kth[, axis, kind, order])	Returns the indices that would partition this array.
`argsort`([axis, kind, order])	Returns the indices that would sort this array.
`astype`(dtype[, order, casting, subok, copy])	Copy of the array, cast to a specified type.
`byteswap`([inplace])	Swap the bytes of the array elements

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Table 2 – continued from previous page

`choose`(choices[, out, mode])	Use an index array to construct a new array from a set of choices.
`clip`([min, max, out])	Return an array whose values are limited to `[min, max]`.
`compress`(condition[, axis, out])	Return selected slices of this array along given axis.
`conj`()	Complex-conjugate all elements.
`conjugate`()	Return the complex conjugate, element-wise.
`copy`([order])	Return a copy of the array.
`cumprod`([axis, dtype, out])	Return the cumulative product of the elements along the given axis.
`cumsum`([axis, dtype, out])	Return the cumulative sum of the elements along the given axis.
`derivative`([x, Y])	If `differentiator` or `jacobinator` is set, this returns the derivative of the `Field`.
`diagonal`([offset, axis1, axis2])	Return specified diagonals.
`dot`(b[, out])	Dot product of two arrays.
`dump`(file)	Dump a pickle of the array to the specified file.
`dumps`()	Returns the pickle of the array as a string.
`fill`(value)	Fill the array with a scalar value.
`flatten`([order])	Return a copy of the array collapsed into one dimension.
`getfield`(dtype[, offset])	Returns a field of the given array as a certain type.
`item`(*args)	Copy an element of an array to a standard Python scalar and return it.
`itemset`(*args)	Insert scalar into an array (scalar is cast to array's dtype, if possible)
`jacobian`([x])	If `jacobinator` is set, this returns the Jacobi matrix of the `Field`.
`max`([axis, out, keepdims, initial, where])	Return the maximum along a given axis.
`mean`([axis, dtype, out, keepdims, where])	Returns the average of the array elements along given axis.
`min`([axis, out, keepdims, initial, where])	Return the minimum along a given axis.
`newbyteorder`([new_order])	Return the array with the same data viewed with a different byte order.
`nonzero`()	Return the indices of the elements that are non-zero.
`partition`(kth[, axis, kind, order])	Rearranges the elements in the array in such a way that the value of the element in kth position is in the position it would be in a sorted array.
`prod`([axis, dtype, out, keepdims, initial, ...])	Return the product of the array elements over the given axis
`ptp`([axis, out, keepdims])	Peak to peak (maximum - minimum) value along a given axis.
`put`(indices, values[, mode])	Set `a.flat[n] = values[n]` for all *n* in indices.
`ravel`([order])	Return a flattened array.
`repeat`(repeats[, axis])	Repeat elements of an array.
`reshape`(shape[, order])	Returns an array containing the same data with a new shape.
`resize`(new_shape[, refcheck])	Change shape and size of array in-place.
`round`([decimals, out])	Return *a* with each element rounded to the given number of decimals.

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Table 2 – continued from previous page

searchsorted(v[, side, sorter])	Find indices where elements of v should be inserted in a to maintain order.
setfield(val, dtype[, offset])	Put a value into a specified place in a field defined by a data-type.
setflags([write, align, uic])	Set array flags WRITEABLE, ALIGNED, (WRITEBACKIFCOPY and UPDATEIFCOPY), respectively.
sort([axis, kind, order])	Sort an array in-place.
squeeze([axis])	Remove axes of length one from *a*.
std([axis, dtype, out, ddof, keepdims, where])	Returns the standard deviation of the array elements along given axis.
suggest(value[, reset])	Suggest a step size
sum([axis, dtype, out, keepdims, initial, where])	Return the sum of the array elements over the given axis.
swapaxes(axis1, axis2)	Return a view of the array with *axis1* and *axis2* interchanged.
take(indices[, axis, out, mode])	Return an array formed from the elements of *a* at the given indices.
tobytes([order])	Construct Python bytes containing the raw data bytes in the array.
tofile(fid[, sep, format])	Write array to a file as text or binary (default).
tolist()	Return the array as an a.ndim-levels deep nested list of Python scalars.
tostring([order])	A compatibility alias for *tobytes*, with exactly the same behavior.
trace([offset, axis1, axis2, dtype, out])	Return the sum along diagonals of the array.
transpose(*axes)	Returns a view of the array with axes transposed.
update()	Not used for IntVar.
var([axis, dtype, out, ddof, keepdims, where])	Returns the variance of the array elements, along given axis.
view([dtype][, type])	New view of array with the same data.

Attributes Summary

maxstepsize	Maximum possible step size, i.e., to next snapshot.
nextsnapshot	Value of the next snapshot.
prevsnapshot	Value of the previous snapshot.
prevstepsize	Previously taken step size.
snapshots	Snapshots at which output should be written.
stepsize	Current stepsize.
suggested	Suggested step size.

Methods Summary

suggest(value[, reset])	Suggest a step size
update()	Not used for `IntVar`.

Attributes Documentation

maxstepsize

Maximum possible step size, i.e., to next snapshot.

nextsnapshot

Value of the next snapshot.

prevsnapshot

Value of the previous snapshot.

prevstepsize

Previously taken step size.

snapshots

Snapshots at which output should be written.

Even if no outputs are written it needs to contain at least one value that specifies the end point of the simulation.

stepsize

Current stepsize.

suggested

Suggested step size.

Methods Documentation

suggest(*value*, *reset=False*)

Suggest a step size

For adaptive integration schemes, this function can be used to suggest a step size for the next integration step. If many vaiables are integrated this safes the smallest suggested step size in a temporary buffer accessible via `IntVar.suggested`.

Parameters

- **value** (`Field`) – Suggested step size
- **reset** (*boolean, optional, default : False*) – If True, the previous value will be discarded.

update()

Not used for `IntVar`.

Updater

class simframe.frame.**Updater**(*func=None*)

Bases: object

Class that manages how a Group or Field is updated.

Methods

update(owner, *args, **kwargs)	Function that is called when Group or Field to which Updater belongs is being updated.

Methods Summary

update(owner, *args, **kwargs)	Function that is called when Group or Field to which Updater belongs is being updated.

Methods Documentation

update(*owner*, **args*, ***kwargs*)

Function that is called when Group or Field to which Updater belongs is being updated.

Parameters

- **owner** (Frame) – Parent Frame object
- **args** (*additional positional arguments*) –
- **kwargs** (*additonal keyword arguments*) –

12.2 simframe.integration Package

This package contains infrastructure for solving differential equations within simframe. The Integrator class is the basic class that advances the simulation from snapshot to snapshot by executing one integration Instruction at a time. Instructions contain a list of integration Scheme. The schemes package contains pre-defined integration schemes that are ready to use in simframe.

12.2.1 Classes

Instruction(scheme, Y[, fstep, controller, ...])	Integration Instruction that controls the execution of an integration Scheme.
Integrator(var[, instructions, failop, ...])	Integrator class that manages the integration instructions
Scheme(scheme[, controller, description])	Class for an integration Scheme that can be used as template for creating custom schemes.

Instruction

class simframe.integration.**Instruction**(*scheme*, *Y*, *fstep=1.0*, *controller={}*, *description=''*)

Bases: *Scheme*

Integration `Instruction` that controls the execution of an integration `Scheme`.

Attributes

Y
The `Field` to be integrated

controller
Dictionary with keyword arguments that is passed to the integration `Scheme`.

description
Description of the `Scheme`.

fstep
Fraction of step size the `Scheme` will be applied to `Field`

scheme
Integration `Scheme`.

Methods

__call__([dx])	Execution of the integration instruction

Attributes Summary

Y	The `Field` to be integrated
fstep	Fraction of step size the `Scheme` will be applied to `Field`

Methods Summary

__call__([dx])	Execution of the integration instruction

Attributes Documentation

Y

The `Field` to be integrated

fstep

Fraction of step size the `Scheme` will be applied to `Field`

Methods Documentation

__call__(*dx=None*)

Execution of the integration instruction

Parameters

dx (`IntVar, optional, default : None`) – Stepsize of the integration variable

Returns

Y1 – New value of the variable to be integrated

Return type

Field

Integrator

class `simframe.integration.`**Integrator**(*var*, *instructions=[]*, *failop=None*, *preparator=None*, *finalizer=None*, *maxit=500*, *description=''*)

Bases: `object`

`Integrator` class that manages the integration instructions

Attributes

description

Description of integrator

failop

`Heartbeat` objects that is called if any integration `Instruction` returned `False`

finalizer

`Heartbeat` object that is called after the integration was successful.

instructions

List of integration `Instructions` that will be executed in that order.

maxit

Maximum number of integration tries until program will be aborted.

preparator

`Heartbeat` object that is called before the integration instructions will be executed.

var

The integration variable `IntVar` that is associated with this `Integrator`.

Methods

integrate()	Method that executes one integration step.

Attributes Summary

description	Description of integrator
failop	`Heartbeat` objects that is called if any integration `Instruction` returned `False`
finalizer	`Heartbeat` object that is called after the integration was successful.
instructions	List of integration `Instructions` that will be executed in that order.
maxit	Maximum number of integration tries until program will be aborted.
preparator	`Heartbeat` object that is called before the integration instructions will be executed.
var	The integration variable `IntVar` that is associated with this `Integrator`.

Methods Summary

integrate()	Method that executes one integration step.

Attributes Documentation

description

Description of integrator

failop

`Heartbeat` objects that is called if any integration `Instruction` returned `False`

finalizer

`Heartbeat` object that is called after the integration was successful.

instructions

List of integration `Instructions` that will be executed in that order.

maxit

Maximum number of integration tries until program will be aborted.

preparator

`Heartbeat` object that is called before the integration instructions will be executed.

var

The integration variable `IntVar` that is associated with this `Integrator`.

Methods Documentation

integrate()

Method that executes one integration step.

Scheme

class simframe.integration.**Scheme**(*scheme*, *controller={}*, *description=''*)

Bases: object

Class for an integration Scheme that can be used as template for creating custom schemes.

Notes

The integration Scheme needs to return False if the integration failed. The Integrator will then perform a fail operation and will try it again. This can be used to implement schemes with adaptive step sizes. If the step size was not small enough the fail operation can reduce it further.

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

__call__(x0, Y0, dx, *args, **kwargs)	Method for returning the new value of the variable to be integrated.

Attributes Summary

controller	Dictionary with keyword arguments that is passed to the integration Scheme.
description	Description of the Scheme.
scheme	Integration Scheme.

Methods Summary

__call__(x0, Y0, dx, *args, **kwargs)	Method for returning the new value of the variable to be integrated.

Attributes Documentation

controller

Dictionary with keyword arguments that is passed to the integration `Scheme`.

description

Description of the `Scheme`.

scheme

Integration `Scheme`.

Methods Documentation

__call__(*x0*, *Y0*, *dx*, **args*, ***kwargs*)

Method for returning the new value of the variable to be integrated.

Parameters

- **x0** (*Intvar*) – Integration variable at beginning of scheme
- **Y0** (`Field`) – Variable to be integrated at the beginning of scheme
- **dx** (`IntVar`) – Stepsize of integration variable
- **controller** (*dict, optional, default : {}*) – Additional keyword arguments passed to integration scheme
- **args** (*additional positional arguments*) –
- **kwargs** (*additional kewyowrd arguments*) –

Returns

Y1 – New value of the variable to be integrated. Functions needs to return `False` if integration failed.

Return type

Field or False

12.3 simframe.integration.schemes Package

This package contains pre-defined instances of integration schemes that can be used in `simframe`. The naming convention is `<expl/impl>_<order>_<name>(<_additonal>)`.

For example: The fifth-order adaptive Cash-Karp scheme is `expl_5_cash_karp_adptv`, the 1st-order implicit Euler scheme using a GMRES solver is `impl_1_euler_gmres`.

12.3.1 Classes

expl_1_euler(*args, **kwargs)	Class for explicit 1st-order Euler method
expl_2_fehlberg_adptv(*args, **kwargs)	Class for explicit adaptive 2nd-order Fehlberg's method
expl_2_heun(*args, **kwargs)	Class for explicit 2nd-order Heun's method
expl_2_heun_euler_adptv(*args, **kwargs)	Class for explicit adaptive 2nd-order Heun-Euler method
expl_2_midpoint(*args, **kwargs)	Class for explicit 2nd-order midpoint method
expl_2_ralston(*args, **kwargs)	Class for explicit 2nd-order Ralston's method
expl_3_bogacki_shampine_adptv(*args, **kwargs)	Class for explicit adaptive 3rd-order Bogacki-Shampine method
expl_3_gottlieb_shu_adptv(*args, **kwargs)	Class for explicit adaptive 3rd-order Gottlieb-Shu method
expl_3_heun(*args, **kwargs)	Class for explicit 3rd-order Heun's method
expl_3_kutta(*args, **kwargs)	Class for explicit 3rd-order Kutta's method
expl_3_ralston(*args, **kwargs)	Class for explicit 3rd-order Ralston's method
expl_3_ssprk(*args, **kwargs)	Class for explicit 3rd-order Strong Stability Preserving Runge-Kutta method
expl_4_38rule(*args, **kwargs)	Class for explicit 4th-order 3/8 rule method
expl_4_ralston(*args, **kwargs)	Class for explicit 4th-order Ralston's method
expl_4_runge_kutta(*args, **kwargs)	Class for explicit 4th-order classical Runge-Kutta method
expl_5_cash_karp_adptv(*args, **kwargs)	Class for explicit adaptive 5th-order Cash-Karp method
expl_5_dormand_prince_adptv(*args, **kwargs)	Class for explicit adaptive 5th-order Dormand-Prince method
impl_1_euler_direct(*args, **kwargs)	Class for implicit 1st-order direct Euler method
impl_1_euler_gmres(*args, **kwargs)	Class for implicit 1st-order Euler method with GMRES solver
impl_2_midpoint_direct(*args, **kwargs)	Class for implicit 2nd-order direct midpoint method
update(*args, **kwargs)	Class to update a field after integration.

expl_1_euler

class simframe.integration.schemes.**expl_1_euler**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit 1st-order Euler method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_2_fehlberg_adptv

class simframe.integration.schemes.**expl_2_fehlberg_adptv**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit adaptive 2nd-order Fehlberg's method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_2_heun

class simframe.integration.schemes.**expl_2_heun**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit 2nd-order Heun's method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_2_heun_euler_adptv

class simframe.integration.schemes.**expl_2_heun_euler_adptv**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit adaptive 2nd-order Heun-Euler method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_2_midpoint

class simframe.integration.schemes.**expl_2_midpoint**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit 2nd-order midpoint method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_2_ralston

class simframe.integration.schemes.**expl_2_ralston**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit 2nd-order Ralston's method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_3_bogacki_shampine_adptv

class simframe.integration.schemes.**expl_3_bogacki_shampine_adptv**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit adaptive 3rd-order Bogacki-Shampine method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_3_gottlieb_shu_adptv

class simframe.integration.schemes.**expl_3_gottlieb_shu_adptv**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit adaptive 3rd-order Gottlieb-Shu method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_3_heun

class simframe.integration.schemes.**expl_3_heun**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit 3rd-order Heun's method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_3_kutta

class simframe.integration.schemes.**expl_3_kutta**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit 3rd-order Kutta's method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_3_ralston

class simframe.integration.schemes.**expl_3_ralston**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit 3rd-order Ralston's method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_3_ssprk

class simframe.integration.schemes.**expl_3_ssprk**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit 3rd-order Strong Stability Preserving Runge-Kutta method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_4_38rule

class simframe.integration.schemes.**expl_4_38rule**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit 4th-order 3/8 rule method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_4_ralston

class simframe.integration.schemes.**expl_4_ralston**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit 4th-order Ralston's method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_4_runge_kutta

class simframe.integration.schemes.**expl_4_runge_kutta**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit 4th-order classical Runge-Kutta method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_5_cash_karp_adptv

class simframe.integration.schemes.**expl_5_cash_karp_adptv**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit adaptive 5th-order Cash-Karp method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

expl_5_dormand_prince_adptv

class simframe.integration.schemes.**expl_5_dormand_prince_adptv**(**args*, ***kwargs*)

Bases: *Scheme*

Class for explicit adaptive 5th-order Dormand-Prince method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

impl_1_euler_direct

class simframe.integration.schemes.**impl_1_euler_direct**(**args*, ***kwargs*)

Bases: *Scheme*

Class for implicit 1st-order direct Euler method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

impl_1_euler_gmres

class simframe.integration.schemes.**impl_1_euler_gmres**(**args*, ***kwargs*)

Bases: *Scheme*

Class for implicit 1st-order Euler method with GMRES solver

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the Scheme.

scheme
Integration Scheme.

Methods

impl_2_midpoint_direct

class simframe.integration.schemes.**impl_2_midpoint_direct**(**args*, ***kwargs*)

Bases: *Scheme*

Class for implicit 2nd-order direct midpoint method

Attributes

controller
Dictionary with keyword arguments that is passed to the integration Scheme.

description
Description of the `Scheme`.

scheme
Integration `Scheme`.

Methods

update

class `simframe.integration.schemes.`**update**(**args*, ***kwargs*)

Bases: *Scheme*

Class to update a field after integration.

Attributes

controller
Dictionary with keyword arguments that is passed to the integration `Scheme`.

description
Description of the `Scheme`.

scheme
Integration `Scheme`.

Methods

12.4 simframe.io Package

This package is for input/output operations. It contains template `Writer` and `Reader` classes that can be used to create customized writing and reading methods. The package `writers` contains pre-defined `Writer` instances for writing and reading `simframe` data. The package furthermore contains a method for reading dump files and for printing a progress bar in an interactive shell.

12.4.1 Functions

readdump(filename)	Reads dumpfile and returns `Frame` object

readdump

`simframe.io.readdump(filename)`

Reads dumpfile and returns `Frame` object

Parameters
filename (*str*) – Path to file to be read

Returns
obj – object read from dump file

Return type
object

Notes

Only read dump files from sources you trust. Malware can be injected.

12.4.2 Classes

Reader(writer[, description])	General class for reading output files.
Writer(func[, datadir, filename, zfill, ...])	General class for writing output files.
Progressbar([prefix, suffix, fill, empty, ...])	Class for printing progress bar to terminal.

Reader

class `simframe.io.Reader(writer, description='')`

Bases: `object`

General class for reading output files. Every `Writer` class should also provide a reader for its data files.

Custom `Reader` must provide a method `Reader.output()` that reads a single output file and returns the data set as type `SimpleNamespace`.

The general `Reader` class provides a function that stitches together all `SimpleNamespaces` the `Reader.output()` method provides into a single `SimpleNamespace` by adding another dimension along the integration variable `IntVar`.

Attributes

description
Description of the `Reader`.

Methods

all()	Functions that reads all output files and combines them into a single `SimpleNamespace`.
listfiles()	Method to list all data files in a directory
output(file)	Function that returns the data of a single output file.
sequence(field)	Function that returns the entire sequence of a specific field.

Attributes Summary

description	Description of the `Reader`.

Methods Summary

all()	Functions that reads all output files and combines them into a single `SimpleNamespace`.
listfiles()	Method to list all data files in a directory
output(file)	Function that returns the data of a single output file.
sequence(field)	Function that returns the entire sequence of a specific field.

Attributes Documentation

`description`

Description of the `Reader`.

Methods Documentation

`all()`

Functions that reads all output files and combines them into a single `SimpleNamespace`.

Returns
dataset – Namespace of data set.

Return type
SimpleNamespace

Notes

This function is reading one output files to get the structure of the data and calls `read.sequence()` for every field in the data structure.

`listfiles()`

Method to list all data files in a directory

Returns
files – List of strings of all found data files sorted alphanumerically.

Return type
list

Notes

Function only searches for files that match the pattern specified by the `Writer`'s `filename` and `extension` attributes.

output(*file*)

Function that returns the data of a single output file.

Parameters
file (*str*) – Path to file that should be read.

Returns
data – Data set of a single output file.

Return type
SimpleNamespace

sequence(*field*)

Function that returns the entire sequence of a specific field.

Parameters
field (*str*) – String with location of requested field

Returns
seq – Array with requested values

Return type
array

Notes

`field` is addressing the values just as in the parent frame object. E.g. `"groupA.groupB.fieldC"` is addressing `Frame.groupA.groupB.fieldC`.

Writer

class simframe.io.**Writer**(*func*, *datadir='data'*, *filename='data'*, *zfill=4*, *extension='out'*, *overwrite=False*, *dumping=True*, *reader=None*, *verbosity=1*, *description=''*, *options={}*)

Bases: `object`

General class for writing output files. It should be used as wrapper for customized `Writer`.

Attributes

datadir
Data directory of output files.

description
Description of `Writer`.

dumping
If `True` dump files will be written.

extension
Filename extension of output files.

filename
Base filename of output files.

options
Dictionary of keyword arguments passed to customized writing routine.

overwrite
If `True` existing output files will be overwritten.

read
`Reader` object for reading output files.

verbosity
Verbosity of the writer.

zfill
Zero padding of numbered files names.

Methods

checkdatadir([datadir, createdir])	Function checks if data directory exists and creates it if necessary.
write(owner, i, forceoverwrite[, filename])	Writes output to file
writedump(frame[, filename])	Writes the `Frame` to dump file

Attributes Summary

datadir	Data directory of output files.
description	Description of `Writer`.
dumping	If `True` dump files will be written.
extension	Filename extension of output files.
filename	Base filename of output files.
options	Dictionary of keyword arguments passed to customized writing routine.
overwrite	If `True` existing output files will be overwritten.
read	`Reader` object for reading output files.
verbosity	Verbosity of the writer.
zfill	Zero padding of numbered files names.

Methods Summary

checkdatadir([datadir, createdir])	Function checks if data directory exists and creates it if necessary.
write(owner, i, forceoverwrite[, filename])	Writes output to file
writedump(frame[, filename])	Writes the `Frame` to dump file

Attributes Documentation

datadir

Data directory of output files.

description

Description of `Writer`.

dumping

If `True` dump files will be written.

extension

Filename extension of output files.

filename

Base filename of output files.

options

Dictionary of keyword arguments passed to customized writing routine.

overwrite

If `True` existing output files will be overwritten.

read

`Reader` object for reading output files.

verbosity

Verbosity of the writer.

zfill

Zero padding of numbered files names.

Methods Documentation

checkdatadir(*datadir=None*, *createdir=False*)

Function checks if data directory exists and creates it if necessary.

Parameters

- **datadir** (*string or None, optinal, default : None*) – Data directory to be checked. If None it assumes the data directory of the parent writer.
- **createdir** (*boolen, optional, default : False*) – If True function creates data directory if it does not exist.

Returns

datadirexists – True if directory exists, False if not

Return type

boolean

write(*owner*, *i*, *forceoverwrite*, *filename=''*)

Writes output to file

Parameters

- **owner** (`Frame`) – Parent `Frame` object
- **i** (*int*) – Number of output

- **forceoverwrite** (*boolean*) – If `True` it will forces and overwrite of the file if it exists independent of the writer attribute
- **filename** (*string*) – If this is not "" the writer will use this filename instead of the standard scheme

writedump(*frame*, *filename=''*)

Writes the `Frame` to dump file

Parameters

- **frame** (*object*) – object to be written to file
- **filename** (*str, optional, default : ""*) – path to file to be written if not set, filename will be <writer.datadir>/frame.dmp.

Progressbar

class simframe.io.**Progressbar**(*prefix=' '*, *suffix='| '*, *fill=''*, *empty=' '*, *length=25*, *color='blue'*, *spinner=None*)

Bases: `object`

Class for printing progress bar to terminal.

Methods

__call__(x, x0, x1, s0, s1)	Prints the current progress bar.
print(x, x0, x1, s0, s1)	Function prints the current progress bar.

Methods Summary

__call__(x, x0, x1, s0, s1)	Prints the current progress bar.
print(x, x0, x1, s0, s1)	Function prints the current progress bar.

Methods Documentation

__call__(*x*, *x0*, *x1*, *s0*, *s1*)

Prints the current progress bar.

Parameters

- **x** (*Number*) – Current state of progress
- **x0** (*Number*) – Starting point of snapshot
- **x1** (*Number*) – End point of snapshot
- **s0** (*Number*) – Starting point of simulation
- **s1** (*Number*) – End point of simulation

print(*x*, *x0*, *x1*, *s0*, *s1*)

Function prints the current progress bar. If the end of either the snapshot or the simulation is reached, no progress bar will be printed.

Parameters

- **x** (*Number*) – Current state of progress
- **x0** (*Number*) – Starting point of snapshot
- **x1** (*Number*) – End point of snapshot
- **s0** (*Number*) – Starting point of simulation
- **s1** (*Number*) – End point of simulation

12.5 simframe.io.writers Package

This package contains pre-defined `Writer` instances that can be used for writing and reading `Frame` objects. The `hdf5writer` writes data files in the HDF5 file format. The `namespacewriter` does not write output files (except for dump files if required). The data is stored locally in the `Writer` object itself.

12.5.1 Classes

hdf5writer(*args, **kwargs)	Class for writing HDF5 output files.
namespacewriter(*args, **kwargs)	Class to write `Frame` object to namespace

hdf5writer

class simframe.io.writers.**hdf5writer**(**args*, ***kwargs*)

Bases: *Writer*

Class for writing HDF5 output files.

Attributes

datadir
Data directory of output files.

description
Description of `Writer`.

dumping
If `True` dump files will be written.

extension
Filename extension of output files.

filename
Base filename of output files.

options
Dictionary of keyword arguments passed to customized writing routine.

overwrite
If `True` existing output files will be overwritten.

read
`Reader` object for reading output files.

verbosity
Verbosity of the writer.

zfill
Zero padding of numbered files names.

Methods

namespacewriter

class `simframe.io.writers.`**`namespacewriter`**(**args*, ***kwargs*)

Bases: *Writer*

Class to write `Frame` object to namespace

Attributes

datadir
Data directory of output files.

description
Description of `Writer`.

dumping
If `True` dump files will be written.

extension
Filename extension of output files.

filename
Base filename of output files.

options
Dictionary of keyword arguments passed to customized writing routine.

overwrite
If `True` existing output files will be overwritten.

read
`Reader` object for reading output files.

verbosity
Verbosity of the writer.

zfill
Zero padding of numbered files names.

Methods

Methods Summary

`reset()`	This resets the namespace.
`write`(owner[, i])	Writes output to namespace

Methods Documentation

`reset()`

This resets the namespace.

Notes

WARNING: This cannot be undone.

`write`(*owner*, *i=0*, **args*, ***kwargs*)

Writes output to namespace

Parameters

- **`owner`** (`Frame`) – Parent frame object
- **`i`** (*`int`*) – Not used in this class
- **`forceoverwrite`** (*`boolean`*) – Not used in this class
- **`filename`** (*`string`*) – Not used in this class

12.6 simframe.utils Package

Package contains utility classes that facilitate the use of `simframe`

`Color` is a generic class that can be used to colorize text. `colorize` is an instance of `Color`, that can be called to add decorators to a string for colored output.

12.6.1 Functions

`byteformat`(b)	Function returns a formatted string for given memory usage.

byteformat

`simframe.utils.byteformat(b)`

Function returns a formatted string for given memory usage.

Parameters
b (*float*) – Memory usage in bytes

Returns
s – Formatted string of memory usage

Return type
string

12.6.2 Classes

Color([color])	Class to decorate strings with color tags.

Color

class `simframe.utils.Color(color='reset')`

Bases: `object`

Class to decorate strings with color tags.

Attributes

color
Of type `Color` with color information.

Methods

__call__(s[, color])	Colorizes string

Attributes Summary

color	Of type `Color` with color information.

Methods Summary

__call__(s[, color])	Colorizes string

Attributes Documentation

color

Of type `Color` with color information.

Methods Documentation

__call__(*s*, *color=None*)

Colorizes string

Parameters

- **s** (*string*) – String to be colorized
- **color** (*string, optional, default : None*) – Color used to colorize. If None, standard color is used

Returns

cstr – Colorized string

Return type

string

CHAPTER

THIRTEEN

INDICES AND TABLES

- genindex
- modindex
- search

PYTHON MODULE INDEX

S

INDEX

Symbols

A

B

C

D

E

F

V

W

Y

Z