PyElastica

Release 0.2.3

Gazzola Lab

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ELASTICA OVERVIEW

Elastica is a *free* and *open-source* software project for the simulation of assemblies of slender, one-dimensional structures using Cosserat Rod theory.

More information about Elastica is available at the project website

PYELASTICA

PyElastica is the python implementation of Elastica. The easiest way to install PyElastica is with PIP:

```
$ pip install pyelastica
```

Or download the source code from the GitHub repo

1.1 Elastica++

Elastica++ is a C++ implementation of Elastica. The expected release date for the beta version is 2022 Q2.

COMMUNITY

We mainly use git-issue to communicate the roadmap, updates, helps, and bug fixes. If you have problem using PyElastica, check if similar issue is reported in git-issue.

We also opened *gitter* channel for short and immediate feedbacks.

CONTRIBUTING

If you are interested to contribute, please read contribution-guide first.

3.1 About

Elastica is a *free* and *open-source* software project for the simulation of assemblies of slender one-dimensional bodies using Cosserat Rod theory. It has been designed to be modular, extensible and easy to use. It allows the user to define a collection of Cosserat rods subject to both external (i.e. gravity, friction, etc...) and internal (i.e. muscle torque) forces. Rods account for self-contact and can be combined to create assemblies of rods, which can then be used to model increasingly complex system.

For more information on Elastica and Cosserat rods, see the project website https://cosseratrods.org

Elastica is developed and maintained by the Gazzola Lab at the University of Illinois at Urbana-Champaign. For more information on the projects we work on, see https://mattia-lab.com.

Funding for the development of Elastica has been provided by:

3.2 Installation

3.2.1 Instruction

PyElastica requires Python 3.5 - 3.8, which needs to be installed prior to using PyElastica. For information on installing Python, see here. If you are interested in using a package manager like Conda, see here.

Note: Python version above 3.8 is tested only in Ubuntu and Mac OS. For Windows 10, some of the dependencies were not yet compatible.

The easiest way to install PyElastica is with `pip`:

```
$ pip install pyelastica
```

You can also download the source code for PyElastica directly from GitHub.

3.2.2 Dependencies

The core of PyElastica is developed using:

- numpy

- numba

- scipy

- tqdm

- matplotlib (visualization)

Above packages will be installed along with PyElastica if you used `pip` to install. If you have directly downloaded the source code, you must install these packages separately.

3.3 Workflow

When using PyElastica, users will setup a simulation in which they define a system of rods, define initial and boundary conditions on the rods, run the simulation, and then post-process the results. Here, we outline a typical template of using PyElastica.

Important: A note on notation: Like other FEA packages such as Abaqus, PyElastica does not enforce units. This means that you are required to make sure that all units for your input variables are consistent. When in doubt, SI units are always safe, however, if you have a very small length scale ($\sim$ nm), then you may need to rescale your units to avoid needing prohibitively small time steps and/or roundoff errors.

```python
from elastica.wrappers import (
    BaseSystemCollection,
    Connections,
    Constraints,
    Forcing,
    CallBacks
)

class SystemSimulator(
    BaseSystemCollection,
    Constraints, # Enabled to use boundary conditions 'OneEndFixedBC'
    Forcing,     # Enabled to use forcing 'GravityForces'
    Connections, # Enabled to use FixedJoint
    CallBacks    # Enabled to use callback
):
    pass
```

This simply combines all the wrappers previously imported together. If a wrapper is not needed for the simulation, it does not need to be added here.

Available components are:

Component	Note
BaseSystemCollection	**Required** for all simulator.
Constraints	
Forcing	
Connections	
CallBacks	

Note: We adopted a composition and mixin design paradigm in building elastica. The detail of the implementation is not important in using the package, but we left some references to read *here*.

```python
from elastica.rod.cosserat_rod import CosseratRod

# Create rod
direction = np.array([0.0, 0.0, 1.0])
normal = np.array([0.0, 1.0, 0.0])
rod1 = CosseratRod.straight_rod(
    n_elements=50,                          # number of elements
    start=np.array([0.0, 0.0, 0.0]),        # Starting position of first node in
→rod
    direction=direction,                    # Direction the rod extends
    normal=normal,                          # normal vector of rod
    base_length=0.5,                        # original length of rod (m)
    base_radius=10e-2,                      # original radius of rod (m)
    density=1e3,                            # density of rod (kg/m^3)
    nu=1e-3,                                # Energy dissipation of rod
    youngs_modulus=1e7,                     # Elastic Modulus (Pa)
    poisson_ratio=0.5,                      # Poisson Ratio
)
rod2 = CosseratRod.straight_rod(
    n_elements=50,                          # number of elements
    start=np.array([0.0, 0.0, 0.5]),        # Starting position of first node in
→rod
    direction=direction,                    # Direction the rod extends
    normal=normal,                          # normal vector of rod
    base_length=0.5,                        # original length of rod (m)
    base_radius=10e-2,                      # original radius of rod (m)
    density=1e3,                            # density of rod (kg/m^3)
    nu=1e-3,                                # Energy dissipation of rod
    youngs_modulus=1e7,                     # Elastic Modulus (Pa)
    poisson_ratio=0.5,                      # Poisson Ratio
)

# Add rod to SystemSimulator
SystemSimulator.append(rod1)
SystemSimulator.append(rod2)
```

This can be repeated to create multiple rods. Supported geometries are listed in *API documentation*.

Note: The number of element (`n_elements`) and `base_length` determines the spatial discretization `dx`. More detail discussion is included *here*.

Now that we have added all our rods to `SystemSimulator`, we need to apply the relevant boundary conditions. See *this page* for in-depth explanations and documentation.

As a simple example, to fix one end of a rod, we use the `OneEndFixedBC` boundary condition (which we imported in step 1 and apply it to the rod. Here we will be fixing the 0th node as well as the 0th element.

```python
from elastica.boundary_conditions import OneEndFixedBC

SystemSimulator.constrain(rod1).using(
    OneEndFixedBC,                      # Displacement BC being applied
    constrained_position_idx=(0,),     # Node number to apply BC
    constrained_director_idx=(0,)      # Element number to apply BC
)
```

We have now fixed one end of the rod while leaving the other end free. We can also apply forces to free end using the `EndpointForces`. We can also add more complex forcings, such as friction, gravity, or torque throughout the rod. See *this page* for in-depth explanations and documentation.

```python
from elastica.external_forces import EndpointForces

#Define 1x3 array of the applied forces
origin_force = np.array([0.0, 0.0, 0.0])
end_force = np.array([-15.0, 0.0, 0.0])
SystemSimulator.add_forcing_to(rod1).using(
    EndpointForces,                    # Traction BC being applied
    origin_force,                      # Force vector applied at first node
    end_force,                         # Force vector applied at last node
    ramp_up_time=final_time / 2.0      # Ramp up time
)
```

One last condition we can define is the connections between rods. See *this page* for in-depth explanations and documentation.

```python
from elastica.connections import FixedJoint

# Connect rod 1 and rod 2. '_connect_idx' specifies the node number that
# the connection should be applied to. You are specifying the index of a
# list so you can use -1 to access the last node.
SystemSimulator.connect(
    first_rod  = rod1,
    second_rod = rod2,
    first_connect_idx  = -1, # Connect to the last node of the first rod.
    second_connect_idx =  0  # Connect to first node of the second rod.
    ).using(
        FixedJoint,  # Type of connection between rods
        k  = 1e5,    # Spring constant of force holding rods together (F = k*x)
        nu = 0,      # Energy dissipation of joint
        kt = 5e3     # Rotational stiffness of rod to avoid rods twisting
        )
```

If you want to know what happens to the rod during the course of the simulation, you must collect data during the simulation. Here, we demonstrate how the callback function can be defined to export the data you need. There is a base class `CallBackBaseClass` that can help with this.

Note: PyElastica **does not automatically saves** the simulation result. If you do not define a callback function, you will only have the final state of the system at the end of the simulation.

```python
from elastica.callback_functions import CallBackBaseClass

# MyCallBack class is derived from the base call back class.
class MyCallBack(CallBackBaseClass):
    def __init__(self, step_skip: int, callback_params):
        CallBackBaseClass.__init__(self)
        self.every = step_skip
        self.callback_params = callback_params

    # This function is called every time step
    def make_callback(self, system, time, current_step: int):
        if current_step % self.every == 0:
            # Save time, step number, position, orientation and velocity
            self.callback_params["time"].append(time)
            self.callback_params["step"].append(current_step)
            self.callback_params["position" ].append(system.position_collection.copy())
            self.callback_params["directors"].append(system.director_collection.copy())
            self.callback_params["velocity" ].append(system.velocity_collection.copy())
            return

# Create dictionary to hold data from callback function
callback_data_rod1, callback_data_rod2 = defaultdict(list), defaultdict(list)

# Add MyCallBack to SystemSimulator for each rod telling it how often to save data (step_
↪skip)
SystemSimulator.collect_diagnostics(rod1).using(
    MyCallBack, step_skip=1000, callback_params=callback_data_rod1)
SystemSimulator.collect_diagnostics(rod2).using(
    MyCallBack, step_skip=1000, callback_params=callback_data_rod2)
```

You can define different callback functions for different rods and also have different data outputted at different time step intervals depending on your needs. See *this page* for more in-depth documentation.

Now that we have finished defining our rods, the different boundary conditions and connections between them, and how often we want to save data, we have finished setting up the simulation. We now need to finalize the simulator by calling

```python
SystemSimulator.finalize()
```

This goes through and collects all the rods and applied conditions, preparing the system for the simulation.

With our system now ready to be run, we need to define which time stepping algorithm to use. Currently, we suggest using the position Verlet algorithm. We also need to define how much time we want to simulate as well as either the time step (dt) or the number of total time steps we want to take. Once we have defined these things, we can run the simulation by calling `integrate()`, which will start the simulation.

We are still actively testing different integration and time-stepping techniques,

---

`PositionVerlet` is the best default at this moment.

```python
from elastica.timestepper.symplectic_steppers import PositionVerlet
from elastica.timestepper import integrate

timestepper = PositionVerlet()
final_time = 10    # seconds
dt = 1e-5          # seconds
total_steps = int(final_time / dt)
integrate(timestepper, SystemSimulator, final_time, total_steps)
```

More documentation on timestepper and integrator is included *here*

Once the simulation ends, it is time to analyze the data. If you defined a callback function, the data you outputted in available there (i.e. `callback_data_rod1`), otherwise you can access the final configuration of your system through your rod objects. For example, if you want the final position of one of your rods, you can get it from `rod1.position_collection[:]`.

3.4 Discretization

To help get you started building initial intuition about PyElastica, here are some general rules of thumb to follow.

Important: These are based on general observations of how simulations tend to behave and are not guaranteed to always hold. Particularly for choosing dx and dt, it is important to perform a separate convergence study for your specific case.

3.4.1 Number of elements per rod

Generally, the more flexible your rod, the more elements you need. It is important to always perform a convergence test for your simulation, however, 30-50 elements per rod is a good starting point.

3.4.2 Choosing your dx and dt

Generally you will set your dx and then choose a stable dt. Your dx will be a combination of your problems length scale and the number of elements you want. Recall that units can be rescaled as long as they are consistent. If you have have a small rod, selecting a dx on the order of nm without scaling is 1e-9. This small value can cause numerical issues, so it is better to rescale your units so that nm $\sim O(1)$.

When choosing your time step, there are a number of different conditions that can affect your choice. The most important consideration is that the time stepping algorithm remain stable. As a useful heuristic, we have found that dt = 0.01 dx s/m tends to yield stable time steps, but depending on your problem this may not hold. If you wish to be able to resolve the propagation of different waves, then you need to make sure your dt is able to capture their propagation ($dt = dx\sqrt{\rho/G}$ for shear waves or $dt = dx\sqrt{\rho/E}$ for flexural waves).

3.4.3 Run time scaling

PyElastica will scale linearly with the number of time steps, so if you halve your time step, your simulation will take twice as long to finish.

The algorithms that PyElastica is based on scale linearly with the number of elements. However, due to overhead from calling functions in Python, PyElastica does not currently have a strong dependence on the number of nodes. Doubling the number of nodes may only lead to a 10-20% increase in run time. While this means you can decrease your dx without a large run time penalty, remember that you also need to adjust your dt, which will affect the run time.

Adding additional interactions with the environment, such as friction or gravity, will increase run time. Most of these interactions only have a small effect on run time except for rod collision and/or self-intersection. As implemented, these are expensive routines ($O(N^2)$) and should be avoided if possible as they will substantially lengthen your run time.

We are working to add parallel and HPC capabilities to PyElastica. If you are interested in helping us implement these changes, let us know.

3.5 Example Cases

Example cases are the demonstration of physical example with known analytical solution or well-studied phenomenon. Each cases follows the recommended workflow, shown *here*. Feel free to use them as an initial template to build your own case study.

3.5.1 Axial Stretching

```
1    """ Axial stretching test-case
2
3        Assume we have a rod lying aligned in the x-direction, with high internal
4        damping.
5
6        We fix one end (say, the left end) of the rod to a wall. On the right
7        end we apply a force directed axially pulling the rods tip. Linear
8        theory (assuming small displacements) predict that the net displacement
9        experienced by the rod tip is x = FL/AE where the symbols carry their
10       usual meaning (the rod is just a linear spring). We compare our results
11       with the above result.
12
13       We can "improve" the theory by having a better estimate for the rod's
14       spring constant by assuming that it equilibriates under the new position,
15       with
16       x = F * (L + x)/ (A * E)
17       which results in x = (F*l)/(A*E - F). Our rod reaches equilibrium wrt to
18       this position.
19
20       Note that if the damping is not high, the rod oscillates about the eventual
21       resting position (and this agrees with the theoretical predictions without
22       any damping : we should see the rod oscillating simple-harmonically in time).
23
24       isort:skip_file
25   """
26   # FIXME without appending sys.path make it more generic
27   import sys
```

(continues on next page)

```
28
29  sys.path.append("../../")  # isort:skip
30
31  # from collections import defaultdict
32
33  # import numpy as np
34  from matplotlib import pyplot as plt
35
36  from elastica import *
37
38
39  class StretchingBeamSimulator(BaseSystemCollection, Constraints, Forcing, CallBacks):
40      pass
41
42
43  stretch_sim = StretchingBeamSimulator()
44  final_time = 20.0
45
46  # Options
47  PLOT_FIGURE = True
48  SAVE_FIGURE = False
49  SAVE_RESULTS = False
50
51  # setting up test params
52  n_elem = 19
53  start = np.zeros((3,))
54  direction = np.array([1.0, 0.0, 0.0])
55  normal = np.array([0.0, 1.0, 0.0])
56  base_length = 1.0
57  base_radius = 0.025
58  base_area = np.pi * base_radius ** 2
59  density = 1000
60  nu = 2.0
61  youngs_modulus = 1e4
62  # For shear modulus of 1e4, nu is 99!
63  poisson_ratio = 0.5
64
65  stretchable_rod = CosseratRod.straight_rod(
66      n_elem,
67      start,
68      direction,
69      normal,
70      base_length,
71      base_radius,
72      density,
73      nu,
74      youngs_modulus,
75      poisson_ratio,
76  )
77
78  stretch_sim.append(stretchable_rod)
79  stretch_sim.constrain(stretchable_rod).using(
```

```python
80        OneEndFixedBC, constrained_position_idx=(0,), constrained_director_idx=(0,)
81  )
82
83  end_force_x = 1.0
84  end_force = np.array([end_force_x, 0.0, 0.0])
85  stretch_sim.add_forcing_to(stretchable_rod).using(
86      EndpointForces, 0.0 * end_force, end_force, ramp_up_time=1e-2
87  )
88
89  # Add call backs
90  class AxialStretchingCallBack(CallBackBaseClass):
91      """
92      Call back function for continuum snake
93      """
94
95      def __init__(self, step_skip: int, callback_params: dict):
96          CallBackBaseClass.__init__(self)
97          self.every = step_skip
98          self.callback_params = callback_params
99
100      def make_callback(self, system, time, current_step: int):
101
102          if current_step % self.every == 0:
103
104              self.callback_params["time"].append(time)
105              # Collect only x
106              self.callback_params["position"].append(
107                  system.position_collection[0, -1].copy()
108              )
109              return
110
111
112  recorded_history = defaultdict(list)
113  stretch_sim.collect_diagnostics(stretchable_rod).using(
114      AxialStretchingCallBack, step_skip=200, callback_params=recorded_history
115  )
116
117  stretch_sim.finalize()
118  timestepper = PositionVerlet()
119  # timestepper = PEFRL()
120
121  dl = base_length / n_elem
122  dt = 0.01 * dl
123  total_steps = int(final_time / dt)
124  print("Total steps", total_steps)
125  integrate(timestepper, stretch_sim, final_time, total_steps)
126
127  if PLOT_FIGURE:
128      # First-order theory with base-length
129      expected_tip_disp = end_force_x * base_length / base_area / youngs_modulus
130      # First-order theory with modified-length, gives better estimates
131      expected_tip_disp_improved = (
```

```
132            end_force_x * base_length / (base_area * youngs_modulus - end_force_x)
133        )
134
135        fig = plt.figure(figsize=(10, 8), frameon=True, dpi=150)
136        ax = fig.add_subplot(111)
137        ax.plot(recorded_history["time"], recorded_history["position"], lw=2.0)
138        ax.hlines(base_length + expected_tip_disp, 0.0, final_time, "k", "dashdot", lw=1.0)
139        ax.hlines(
140            base_length + expected_tip_disp_improved, 0.0, final_time, "k", "dashed", lw=2.0
141        )
142        if SAVE_FIGURE:
143            fig.savefig("axial_stretching.pdf")
144        plt.show()
145
146 if SAVE_RESULTS:
147     import pickle
148
149     filename = "axial_stretching_data.dat"
150     file = open(filename, "wb")
151     pickle.dump(stretchable_rod, file)
152     file.close()
```

3.5.2 Timoshenko

```
1  __doc__ = """Timoshenko beam validation case, for detailed explanation refer to
2  Gazzola et. al. R. Soc. 2018  section 3.4.3 """
3
4  import numpy as np
5  import sys
6
7  # FIXME without appending sys.path make it more generic
8  sys.path.append("../../")
9  from elastica import *
10 from examples.TimoshenkoBeamCase.timoshenko_postprocessing import plot_timoshenko
11
12
13 class TimoshenkoBeamSimulator(BaseSystemCollection, Constraints, Forcing):
14     pass
15
16
17 timoshenko_sim = TimoshenkoBeamSimulator()
18 final_time = 5000
19
20 # Options
21 PLOT_FIGURE = True
22 SAVE_FIGURE = False
23 SAVE_RESULTS = False
24 ADD_UNSHEARABLE_ROD = True
25
26 # setting up test params
```

```python
n_elem = 100
start = np.zeros((3,))
direction = np.array([0.0, 0.0, 1.0])
normal = np.array([0.0, 1.0, 0.0])
base_length = 3.0
base_radius = 0.25
base_area = np.pi * base_radius ** 2
density = 5000
nu = 0.1
E = 1e6
# For shear modulus of 1e4, nu is 99!
poisson_ratio = 99
shear_modulus = E / (poisson_ratio + 1.0)

shearable_rod = CosseratRod.straight_rod(
    n_elem,
    start,
    direction,
    normal,
    base_length,
    base_radius,
    density,
    nu,
    E,
    shear_modulus=shear_modulus,
)

timoshenko_sim.append(shearable_rod)
timoshenko_sim.constrain(shearable_rod).using(
    OneEndFixedBC, constrained_position_idx=(0,), constrained_director_idx=(0,)
)

end_force = np.array([-15.0, 0.0, 0.0])
timoshenko_sim.add_forcing_to(shearable_rod).using(
    EndpointForces, 0.0 * end_force, end_force, ramp_up_time=final_time / 2.0
)


if ADD_UNSHEARABLE_ROD:
    # Start into the plane
    unshearable_start = np.array([0.0, -1.0, 0.0])
    shear_modulus = E / (-0.7 + 1.0)
    unshearable_rod = CosseratRod.straight_rod(
        n_elem,
        unshearable_start,
        direction,
        normal,
        base_length,
        base_radius,
        density,
        nu,
        E,
```

```python
79          # Unshearable rod needs G -> inf, which is achievable with -ve poisson ratio
80          shear_modulus=shear_modulus,
81      )
82
83      timoshenko_sim.append(unshearable_rod)
84      timoshenko_sim.constrain(unshearable_rod).using(
85          OneEndFixedBC, constrained_position_idx=(0,), constrained_director_idx=(0,)
86      )
87      timoshenko_sim.add_forcing_to(unshearable_rod).using(
88          EndpointForces, 0.0 * end_force, end_force, ramp_up_time=final_time / 2.0
89      )
90
91  timoshenko_sim.finalize()
92  timestepper = PositionVerlet()
93  # timestepper = PEFRL()
94
95  dl = base_length / n_elem
96  dt = 0.01 * dl
97  total_steps = int(final_time / dt)
98  print("Total steps", total_steps)
99  integrate(timestepper, timoshenko_sim, final_time, total_steps)
100
101 if PLOT_FIGURE:
102     plot_timoshenko(shearable_rod, end_force, SAVE_FIGURE, ADD_UNSHEARABLE_ROD)
103
104 if SAVE_RESULTS:
105     import pickle
106
107     filename = "Timoshenko_beam_data.dat"
108     file = open(filename, "wb")
109     pickle.dump(shearable_rod, file)
110     file.close()
```

3.5.3 Butterfly

```python
1  # FIXME without appending sys.path make it more generic
2  import sys
3
4  sys.path.append("../")
5  sys.path.append("../../")
6
7  # from collections import defaultdict
8  import numpy as np
9  from matplotlib import pyplot as plt
10 from matplotlib.colors import to_rgb
11
12
13 from elastica import *
14 from elastica.utils import MaxDimension
15
```

```python
class ButterflySimulator(BaseSystemCollection, CallBacks):
    pass


butterfly_sim = ButterflySimulator()
final_time = 40.0

# Options
PLOT_FIGURE = True
SAVE_FIGURE = True
SAVE_RESULTS = True
ADD_UNSHEARABLE_ROD = False

# setting up test params
# FIXME : Doesn't work with elements > 10 (the inverse rotate kernel fails)
n_elem = 4  # Change based on requirements, but be careful
n_elem += n_elem % 2
half_n_elem = n_elem // 2

origin = np.zeros((3, 1))
angle_of_inclination = np.deg2rad(45.0)

# in-plane
horizontal_direction = np.array([0.0, 0.0, 1.0]).reshape(-1, 1)
vertical_direction = np.array([1.0, 0.0, 0.0]).reshape(-1, 1)

# out-of-plane
normal = np.array([0.0, 1.0, 0.0])

total_length = 3.0
base_radius = 0.25
base_area = np.pi * base_radius ** 2
density = 5000
nu = 0.0
youngs_modulus = 1e4
poisson_ratio = 0.5

positions = np.empty((MaxDimension.value(), n_elem + 1))
dl = total_length / n_elem

# First half of positions stem from slope angle_of_inclination
first_half = np.arange(half_n_elem + 1.0).reshape(1, -1)
positions[..., : half_n_elem + 1] = origin + dl * first_half * (
    np.cos(angle_of_inclination) * horizontal_direction
    + np.sin(angle_of_inclination) * vertical_direction
)
positions[..., half_n_elem:] = positions[
    ..., half_n_elem : half_n_elem + 1
] + dl * first_half * (
    np.cos(angle_of_inclination) * horizontal_direction
    - np.sin(angle_of_inclination) * vertical_direction
```

```
68  )
69
70  butterfly_rod = CosseratRod.straight_rod(
71      n_elem,
72      start=origin.reshape(3),
73      direction=np.array([0.0, 0.0, 1.0]),
74      normal=normal,
75      base_length=total_length,
76      base_radius=base_radius,
77      density=density,
78      nu=nu,
79      youngs_modulus=youngs_modulus,
80      poisson_ratio=poisson_ratio,
81      position=positions,
82  )
83
84  butterfly_sim.append(butterfly_rod)
85
86  # Add call backs
87  class VelocityCallBack(CallBackBaseClass):
88      """
89      Call back function for continuum snake
90      """
91
92      def __init__(self, step_skip: int, callback_params: dict):
93          CallBackBaseClass.__init__(self)
94          self.every = step_skip
95          self.callback_params = callback_params
96
97      def make_callback(self, system, time, current_step: int):
98
99          if current_step % self.every == 0:
100
101              self.callback_params["time"].append(time)
102              # Collect x
103              self.callback_params["position"].append(system.position_collection.copy())
104              # Collect energies as well
105              self.callback_params["te"].append(system.compute_translational_energy())
106              self.callback_params["re"].append(system.compute_rotational_energy())
107              self.callback_params["se"].append(system.compute_shear_energy())
108              self.callback_params["be"].append(system.compute_bending_energy())
109              return
110
111
112  recorded_history = defaultdict(list)
113  # initially record history
114  recorded_history["time"].append(0.0)
115  recorded_history["position"].append(butterfly_rod.position_collection.copy())
116  recorded_history["te"].append(butterfly_rod.compute_translational_energy())
117  recorded_history["re"].append(butterfly_rod.compute_rotational_energy())
118  recorded_history["se"].append(butterfly_rod.compute_shear_energy())
119  recorded_history["be"].append(butterfly_rod.compute_bending_energy())
```

```python
120
121  butterfly_sim.collect_diagnostics(butterfly_rod).using(
122      VelocityCallBack, step_skip=100, callback_params=recorded_history
123  )
124
125
126  butterfly_sim.finalize()
127  timestepper = PositionVerlet()
128  # timestepper = PEFRL()
129
130  dt = 0.01 * dl
131  total_steps = int(final_time / dt)
132  print("Total steps", total_steps)
133  integrate(timestepper, butterfly_sim, final_time, total_steps)
134
135  if PLOT_FIGURE:
136      # Plot the histories
137      fig = plt.figure(figsize=(5, 4), frameon=True, dpi=150)
138      ax = fig.add_subplot(111)
139      positions = recorded_history["position"]
140      # record first position
141      first_position = positions.pop(0)
142      ax.plot(first_position[2, ...], first_position[0, ...], "r--", lw=2.0)
143      n_positions = len(positions)
144      for i, pos in enumerate(positions):
145          alpha = np.exp(i / n_positions - 1)
146          ax.plot(pos[2, ...], pos[0, ...], "b", lw=0.6, alpha=alpha)
147      # final position is also separate
148      last_position = positions.pop()
149      ax.plot(last_position[2, ...], last_position[0, ...], "k--", lw=2.0)
150      # don't block
151      fig.show()
152
153      # Plot the energies
154      energy_fig = plt.figure(figsize=(5, 4), frameon=True, dpi=150)
155      energy_ax = energy_fig.add_subplot(111)
156      times = np.asarray(recorded_history["time"])
157      te = np.asarray(recorded_history["te"])
158      re = np.asarray(recorded_history["re"])
159      be = np.asarray(recorded_history["be"])
160      se = np.asarray(recorded_history["se"])
161
162      energy_ax.plot(times, te, c=to_rgb("xkcd:reddish"), lw=2.0, label="Translations")
163      energy_ax.plot(times, re, c=to_rgb("xkcd:bluish"), lw=2.0, label="Rotation")
164      energy_ax.plot(times, be, c=to_rgb("xkcd:burple"), lw=2.0, label="Bend")
165      energy_ax.plot(times, se, c=to_rgb("xkcd:goldenrod"), lw=2.0, label="Shear")
166      energy_ax.plot(times, te + re + be + se, c="k", lw=2.0, label="Total energy")
167      energy_ax.legend()
168      # don't block
169      energy_fig.show()
170
171      if SAVE_FIGURE:
```

```
172        fig.savefig("butterfly.png")
173        energy_fig.savefig("energies.png")
174
175    plt.show()
176
177 if SAVE_RESULTS:
178    import pickle
179
180    filename = "butterfly_data.dat"
181    file = open(filename, "wb")
182    pickle.dump(butterfly_rod, file)
183    file.close()
```

3.5.4 Helical Buckling

```
1  __doc__ = """Helical buckling validation case, for detailed explanation refer to
2  Gazzola et. al. R. Soc. 2018  section 3.4.1 """
3
4  import numpy as np
5  import sys
6
7  # FIXME without appending sys.path make it more generic
8  sys.path.append("../../")
9  from elastica import *
10 from examples.HelicalBucklingCase.helicalbuckling_postprocessing import (
11     plot_helicalbuckling,
12 )
13
14
15 class HelicalBucklingSimulator(BaseSystemCollection, Constraints, Forcing):
16     pass
17
18
19 helicalbuckling_sim = HelicalBucklingSimulator()
20
21 # Options
22 PLOT_FIGURE = True
23 SAVE_FIGURE = True
24 SAVE_RESULTS = False
25
26 # setting up test params
27 n_elem = 100
28 start = np.zeros((3,))
29 direction = np.array([0.0, 0.0, 1.0])
30 normal = np.array([0.0, 1.0, 0.0])
31 base_length = 100.0
32 base_radius = 0.35
33 base_area = np.pi * base_radius ** 2
34 density = 1.0 / (base_area)
35 nu = 0.01
```

```
36  E = 1e6
37  slack = 3
38  number_of_rotations = 27
39  # For shear modulus of 1e5, nu is 99!
40  poisson_ratio = 9
41  shear_modulus = E / (poisson_ratio + 1.0)
42  shear_matrix = np.repeat(
43      shear_modulus * np.identity((3))[:, :, np.newaxis], n_elem, axis=2
44  )
45  temp_bend_matrix = np.zeros((3, 3))
46  np.fill_diagonal(temp_bend_matrix, [1.345, 1.345, 0.789])
47  bend_matrix = np.repeat(temp_bend_matrix[:, :, np.newaxis], n_elem - 1, axis=2)
48
49  shearable_rod = CosseratRod.straight_rod(
50      n_elem,
51      start,
52      direction,
53      normal,
54      base_length,
55      base_radius,
56      density,
57      nu,
58      E,
59      shear_modulus=shear_modulus,
60  )
61  # TODO: CosseratRod has to be able to take shear matrix as input, we should change it as␣
    ↪done below
62
63  shearable_rod.shear_matrix = shear_matrix
64  shearable_rod.bend_matrix = bend_matrix
65
66
67  helicalbuckling_sim.append(shearable_rod)
68  helicalbuckling_sim.constrain(shearable_rod).using(
69      HelicalBucklingBC,
70      constrained_position_idx=(0, -1),
71      constrained_director_idx=(0, -1),
72      twisting_time=500,
73      slack=slack,
74      number_of_rotations=number_of_rotations,
75  )
76
77  helicalbuckling_sim.finalize()
78  timestepper = PositionVerlet()
79  shearable_rod.velocity_collection[..., int((n_elem) / 2)] += np.array([0, 1e-6, 0.0])
80  # timestepper = PEFRL()
81
82  final_time = 10500.0
83  dl = base_length / n_elem
84  dt = 1e-3 * dl
85  total_steps = int(final_time / dt)
86  print("Total steps", total_steps)
```

```python
87  integrate(timestepper, helicalbuckling_sim, final_time, total_steps)
88
89  if PLOT_FIGURE:
90      plot_helicalbuckling(shearable_rod, SAVE_FIGURE)
91
92  if SAVE_RESULTS:
93      import pickle
94
95      filename = "HelicalBuckling_data.dat"
96      file = open(filename, "wb")
97      pickle.dump(shearable_rod, file)
98      file.close()
```

3.5.5 Continuum Snake

```python
1   __doc__ = """Snake friction case from X. Zhang et. al. Nat. Comm. 2021"""
2
3   import sys
4
5   sys.path.append("../../")
6   from elastica import *
7
8   from examples.ContinuumSnakeCase.continuum_snake_postprocessing import (
9       plot_snake_velocity,
10      plot_video,
11      compute_projected_velocity,
12      plot_curvature,
13  )
14
15
16  class SnakeSimulator(BaseSystemCollection, Constraints, Forcing, CallBacks):
17      pass
18
19
20  def run_snake(
21      b_coeff, PLOT_FIGURE=False, SAVE_FIGURE=False, SAVE_VIDEO=False, SAVE_RESULTS=False
22  ):
23      # Initialize the simulation class
24      snake_sim = SnakeSimulator()
25
26      # Simulation parameters
27      period = 2
28      final_time = (11.0 + 0.01) * period
29      time_step = 8e-6
30      total_steps = int(final_time / time_step)
31      rendering_fps = 60
32      step_skip = int(1.0 / (rendering_fps * time_step))
33
34      # setting up test params
35      n_elem = 50
```

```python
36        start = np.zeros((3,))
37        direction = np.array([0.0, 0.0, 1.0])
38        normal = np.array([0.0, 1.0, 0.0])
39        base_length = 0.35
40        base_radius = base_length * 0.011
41        density = 1000
42        nu = 1e-4
43        E = 1e6
44        poisson_ratio = 0.5
45        shear_modulus = E / (poisson_ratio + 1.0)
46
47        shearable_rod = CosseratRod.straight_rod(
48            n_elem,
49            start,
50            direction,
51            normal,
52            base_length,
53            base_radius,
54            density,
55            nu,
56            E,
57            shear_modulus=shear_modulus,
58        )
59
60        snake_sim.append(shearable_rod)
61
62        # Add gravitational forces
63        gravitational_acc = -9.80665
64        snake_sim.add_forcing_to(shearable_rod).using(
65            GravityForces, acc_gravity=np.array([0.0, gravitational_acc, 0.0])
66        )
67
68        # Add muscle torques
69        wave_length = b_coeff[-1]
70        snake_sim.add_forcing_to(shearable_rod).using(
71            MuscleTorques,
72            base_length=base_length,
73            b_coeff=b_coeff[:-1],
74            period=period,
75            wave_number=2.0 * np.pi / (wave_length),
76            phase_shift=0.0,
77            rest_lengths=shearable_rod.rest_lengths,
78            ramp_up_time=period,
79            direction=normal,
80            with_spline=True,
81        )
82
83        # Add friction forces
84        origin_plane = np.array([0.0, -base_radius, 0.0])
85        normal_plane = normal
86        slip_velocity_tol = 1e-8
87        froude = 0.1
```

```python
88      mu = base_length / (period * period * np.abs(gravitational_acc) * froude)
89      kinetic_mu_array = np.array(
90          [mu, 1.5 * mu, 2.0 * mu]
91      )  # [forward, backward, sideways]
92      static_mu_array = np.zeros(kinetic_mu_array.shape)
93      snake_sim.add_forcing_to(shearable_rod).using(
94          AnisotropicFrictionalPlane,
95          k=1.0,
96          nu=1e-6,
97          plane_origin=origin_plane,
98          plane_normal=normal_plane,
99          slip_velocity_tol=slip_velocity_tol,
100         static_mu_array=static_mu_array,
101         kinetic_mu_array=kinetic_mu_array,
102     )

104     # Add call backs
105     class ContinuumSnakeCallBack(CallBackBaseClass):
106         """
107         Call back function for continuum snake
108         """

110         def __init__(self, step_skip: int, callback_params: dict):
111             CallBackBaseClass.__init__(self)
112             self.every = step_skip
113             self.callback_params = callback_params

115         def make_callback(self, system, time, current_step: int):

117             if current_step % self.every == 0:

119                 self.callback_params["time"].append(time)
120                 self.callback_params["step"].append(current_step)
121                 self.callback_params["position"].append(
122                     system.position_collection.copy()
123                 )
124                 self.callback_params["velocity"].append(
125                     system.velocity_collection.copy()
126                 )
127                 self.callback_params["avg_velocity"].append(
128                     system.compute_velocity_center_of_mass()
129                 )

131                 self.callback_params["center_of_mass"].append(
132                     system.compute_position_center_of_mass()
133                 )
134                 self.callback_params["curvature"].append(system.kappa.copy())

136                 return

138     pp_list = defaultdict(list)
139     snake_sim.collect_diagnostics(shearable_rod).using(
```

```python
140            ContinuumSnakeCallBack, step_skip=step_skip, callback_params=pp_list
141        )
142
143        snake_sim.finalize()
144
145        timestepper = PositionVerlet()
146        integrate(timestepper, snake_sim, final_time, total_steps)
147
148        if PLOT_FIGURE:
149            filename_plot = "continuum_snake_velocity.png"
150            plot_snake_velocity(pp_list, period, filename_plot, SAVE_FIGURE)
151            plot_curvature(pp_list, shearable_rod.rest_lengths, period, SAVE_FIGURE)
152
153            if SAVE_VIDEO:
154                filename_video = "continuum_snake.mp4"
155                plot_video(
156                    pp_list,
157                    video_name=filename_video,
158                    fps=rendering_fps,
159                    xlim=(0, 4),
160                    ylim=(-1, 1),
161                )
162
163        if SAVE_RESULTS:
164            import pickle
165
166            filename = "continuum_snake.dat"
167            file = open(filename, "wb")
168            pickle.dump(pp_list, file)
169            file.close()
170
171        # Compute the average forward velocity. These will be used for optimization.
172        [_, _, avg_forward, avg_lateral] = compute_projected_velocity(pp_list, period)
173
174        return avg_forward, avg_lateral, pp_list
175
176
177    if __name__ == "__main__":
178
179        # Options
180        PLOT_FIGURE = True
181        SAVE_FIGURE = True
182        SAVE_VIDEO = True
183        SAVE_RESULTS = False
184        CMA_OPTION = False
185
186        if CMA_OPTION:
187            import cma
188
189            SAVE_OPTIMIZED_COEFFICIENTS = False
190
191            def optimize_snake(spline_coefficient):
```

```
192            [avg_forward, _, _] = run_snake(
193                spline_coefficient,
194                PLOT_FIGURE=False,
195                SAVE_FIGURE=False,
196                SAVE_VIDEO=False,
197                SAVE_RESULTS=False,
198            )
199            return -avg_forward
200
201        # Optimize snake for forward velocity. In cma.fmin first input is function
202        # to be optimized, second input is initial guess for coefficients you are
    ↪optimizing
203        # for and third input is standard deviation you initially set.
204        optimized_spline_coefficients = cma.fmin(optimize_snake, 7 * [0], 0.5)
205
206        # Save the optimized coefficients to a file
207        filename_data = "optimized_coefficients.txt"
208        if SAVE_OPTIMIZED_COEFFICIENTS:
209            assert filename_data != "", "provide a file name for coefficients"
210            np.savetxt(filename_data, optimized_spline_coefficients, delimiter=",")
211
212    else:
213        # Add muscle forces on the rod
214        if os.path.exists("optimized_coefficients.txt"):
215            t_coeff_optimized = np.genfromtxt(
216                "optimized_coefficients.txt", delimiter=","
217            )
218        else:
219            wave_length = 1.0
220            t_coeff_optimized = np.array(
221                [3.4e-3, 3.3e-3, 4.2e-3, 2.6e-3, 3.6e-3, 3.5e-3]
222            )
223            t_coeff_optimized = np.hstack((t_coeff_optimized, wave_length))
224
225        # run the simulation
226        [avg_forward, avg_lateral, pp_list] = run_snake(
227            t_coeff_optimized, PLOT_FIGURE, SAVE_FIGURE, SAVE_VIDEO, SAVE_RESULTS
228        )
229
230        print("average forward velocity:", avg_forward)
231        print("average forward lateral:", avg_lateral)
```

3.6 Binder Tutorials

We have created several Jupyter notebooks and Python scripts to help get users started with using PyElastica. The Jupyter notebooks are available on Binder, allowing you to try out some of the tutorials without having to install PyElastica.

Note: Additional examples are also available in the examples folder of PyElastica's Github repo.

3.7 Visualization

3.7.1 Matplotlib

If you wish to visualize your system, make sure you define your callback function to output all necessary data. You can either plot your data using a python package such as `matplotlib`, or any rendering software that you choose. Note, many of the visualization scripts in the examples folders require ffmpeg (be sure to install with h264 libraries).

3.7.2 POVray

For high-quality visualization, we suggest POVray. See this tutorial for examples of different ways of visualizing the system.

3.7.3 Rhino

For interactive visualization and rendering, we use Rhino + Grasshopper. See this extension.

3.7.4 VTK

The current version does not have VTK-export capability, although we plan to include this feature later.

3.8 Rods

Base class for rods

class `elastica.rod.rod_base.`**RodBase**
    Base class for all rods.

Notes

All new rod classes must be derived from this RodBase class.

3.8.1 Cosserat Rod

	On Nodes (+1)	On Elements (n_elements)	On Voronoi (-1)
Geometry	position	director, tangents length, rest_length radius volume dilatation	rest voronoi length voronoi dilatation
Kinematics	velocity acceleration external forces damping forces	angular velocity (omega) angular acceleration (alpha) mass second moment of inertia +inverse dilatation rates external torques damping torques	
Elasticity	internal forces	shear matrix (modulus) shear/stretch strain (sigma) rest shear/stretch strain internal torques internal stress	bend matrix (modulus) bend/twist strain (kappa) rest bend/twist strain internal couple
Material	mass	density dissipation constant (force, torque)	

Rod classes and implementation details

```
class elastica.rod.cosserat_rod.CosseratRod(n_elements, position, velocity, omega, acceleration,
                                             angular_acceleration, directors, radius,
                                             mass_second_moment_of_inertia,
                                             inv_mass_second_moment_of_inertia, shear_matrix,
                                             bend_matrix, density, volume, mass,
                                             dissipation_constant_for_forces,
                                             dissipation_constant_for_torques, internal_forces,
                                             internal_torques, external_forces, external_torques,
                                             lengths, rest_lengths, tangents, dilatation, dilatation_rate,
                                             voronoi_dilatation, rest_voronoi_lengths, sigma, kappa,
                                             rest_sigma, rest_kappa, internal_stress, internal_couple,
                                             damping_forces, damping_torques)
```

Cosserat Rod class. This is the preferred class for rods because it is derived from some of the essential base classes.

> **Attributes**
>
> > **n_elems: int** The number of elements of the rod.
> >
> > **position_collection: numpy.ndarray** 2D (dim, n_nodes) array containing data with 'float' type. Array containing node position vectors.
> >
> > **velocity_collection: numpy.ndarray** 2D (dim, n_nodes) array containing data with 'float' type. Array containing node velocity vectors.
> >
> > **acceleration_collection: numpy.ndarray** 2D (dim, n_nodes) array containing data with 'float' type. Array containing node acceleration vectors.
> >
> > **omega_collection: numpy.ndarray** 2D (dim, n_elems) array containing data with 'float' type. Array containing element angular velocity vectors.
> >
> > **alpha_collection: numpy.ndarray** 2D (dim, n_elems) array containing data with 'float' type. Array continging element angular acceleration vectors.
> >
> > **director_collection: numpy.ndarray** 3D (dim, dim, n_elems) array containing data with 'float' type. Array containing element director matrices.
> >
> > **rest_lengths: numpy.ndarray** 1D (n_elems) array containing data with 'float' type. Rod element lengths at rest configuration.
> >
> > **density: numpy.ndarray** 1D (n_elems) array containing data with 'float' type. Rod elements densities.
> >
> > **volume: numpy.ndarray** 1D (n_elems) array containing data with 'float' type. Rod element volumes.
> >
> > **mass: numpy.ndarray** 1D (n_nodes) array containing data with 'float' type. Rod node masses. Note that masses are stored on the nodes, not on elements.
> >
> > **mass_second_moment_of_inertia: numpy.ndarray** 3D (dim, dim, n_elems) array containing data with 'float' type. Rod element mass second moment of interia.
> >
> > **inv_mass_second_moment_of_inertia: numpy.ndarray** 3D (dim, dim, n_elems) array containing data with 'float' type. Rod element inverse mass moment of inertia.
> >
> > **dissipation_constant_for_forces: numpy.ndarray** 1D (n_elems) array containing data with 'float' type. Rod element dissipation coefficient (nu).
> >
> > **dissipation_constant_for_torques: numpy.ndarray** 1D (n_elems) array containing data with 'float' type. Rod element dissipation (nu). Can be customized by passing 'nu_for_torques'.

rest_voronoi_lengths: numpy.ndarray 1D (n_voronoi) array containing data with 'float' type. Rod lengths on the voronoi domain at the rest configuration.

internal_forces: numpy.ndarray 2D (dim, n_nodes) array containing data with 'float' type. Rod node internal forces. Note that internal forces are stored on the node, not on elements.

internal_torques: numpy.ndarray 2D (dim, n_elems) array containing data with 'float' type. Rod element internal torques.

external_forces: numpy.ndarray 2D (dim, n_nodes) array containing data with 'float' type. External forces acting on rod nodes.

external_torques: numpy.ndarray 2D (dim, n_elems) array containing data with 'float' type. External torques acting on rod elements.

lengths: numpy.ndarray 1D (n_elems) array containing data with 'float' type. Rod element lengths.

tangents: numpy.ndarray 2D (dim, n_elems) array containing data with 'float' type. Rod element tangent vectors.

radius: numpy.ndarray 1D (n_elems) array containing data with 'float' type. Rod element radius.

dilatation: numpy.ndarray 1D (n_elems) array containing data with 'float' type. Rod element dilatation.

voronoi_dilatation: numpy.ndarray 1D (n_voronoi) array containing data with 'float' type. Rod dilatation on voronoi domain.

dilatation_rate: numpy.ndarray 1D (n_elems) array containing data with 'float' type. Rod element dilatation rates.

classmethod straight_rod(*n_elements*, *start*, *direction*, *normal*, *base_length*, *base_radius*, *density*, *nu*, *youngs_modulus*, **args*, ***kwargs*)

Cosserat rod constructor for straight-rod geometry.

Parameters

n_elements [int] Number of element. Must be greater than 3. Generarally recommended to start with 40-50, and adjust the resolution.

start [NDArray[3, float]] Starting coordinate in 3D

direction [NDArray[3, float]] Direction of the rod in 3D

normal [NDArray[3, float]] Normal vector of the rod in 3D

base_length [float] Total length of the rod

base_radius [float] Uniform radius of the rod

density [float] Density of the rod

nu [float] Damping coefficient for Rayleigh damping

youngs_modulus [float] Young's modulus

*args [tuple] Additional arguments should be passed as keyword arguments. (e.g. shear_modulus, poisson_ratio)

**kwargs [dict, optional] The "position" and/or "directors" can be overridden by passing "position" and "directors" argument. Remember, the shape of the "position" is (3,n_elements+1) and the shape of the "directors" is (3,3,n_elements).

Returns

> **CosseratRod**

> **Notes**

> Since we expect the Cosserat Rod to simulate soft rod, Poisson's ratio is set to 0.5 by default. It is possible to give additional argument "shear_modulus" or "poisson_ratio" to specify extra modulus.

compute_translational_energy()
> Compute total translational energy of the rod at the instance.

compute_rotational_energy()
> Compute total rotational energy of the rod at the instance.

compute_velocity_center_of_mass()
> Compute velocity center of mass of the rod at the instance.

compute_position_center_of_mass()
> Compute position center of mass of the rod at the instance.

compute_bending_energy()
> Compute total bending energy of the rod at the instance.

compute_shear_energy()
> Compute total shear energy of the rod at the instance.

compute_link(*type_of_additional_segment='next_tangent'*)
> See *Knot Theory (Mixin)* for the detail.

> > **Parameters**

> > > **type_of_additional_segment** [str] Determines the method to compute new segments (elements) added to the rod. Valid inputs are "next_tangent", "end_to_end", "net_tangent", otherwise program uses the center line.

compute_twist()
> See *Knot Theory (Mixin)* for the detail.

compute_writhe(*type_of_additional_segment='next_tangent'*)
> See *Knot Theory (Mixin)* for the detail.

> > **Parameters**

> > > **type_of_additional_segment** [str] Determines the method to compute new segments (elements) added to the rod. Valid inputs are "next_tangent", "end_to_end", "net_tangent", otherwise program uses the center line.

Knot Theory (Mixin)

This script is for computing the link-writhe-twist (LWT) of a rod using the method from Klenin & Langowski 2000 paper. Algorithms are adapted from section S2 of Charles et. al. PRL 2019 paper.

Following example cases includes computing LWT quantities to study the bifurcation:

- Example case (PlectonemesCase)
- Example case (SolenoidCase)

The details discussion is included in N Charles et. al. PRL (2019).

class elastica.rod.knot_theory.**KnotTheoryCompatibleProtocol**(*args*, ***kwds*)
> Required properties to use KnotTheory mixin

class elastica.rod.knot_theory.**KnotTheory**

This mixin should be used in RodBase-derived class that satisfies KnotCompatibleProtocol. The theory behind this module is based on the method from Klenin & Langowski 2000 paper.

KnotTheory can be mixed with any rod-class based on RodBase:

```python
class MyRod(RodBase, KnotTheory):
    def __init__(self):
        super().__init__()
rod = MyRod(...)

total_twist = rod.compute_twist()
total_link = rod.compute_link()
```

There are few alternative way of handling edge-condition in computing Link and Writhe. Here, we provide three methods: "next_tangent", "end_to_end", and "net_tangent". The default *type_of_additional_segment* is set to "next_tangent."

type_of_additional_segment	Description
next_tangent	Adds a two new point at the begining and end of the center line. Distance of these points are given in segment_length. Direction of these points are computed using the rod tangents at the begining and end.
end_to_end	Adds a two new point at the begining and end of the center line. Distance of these points are given in segment_length. Direction of these points are computed using the rod node end positions.
net_tangent	Adds a two new point at the begining and end of the center line. Distance of these points are given in segment_length. Direction of these points are point wise avarege of nodes at the first and second half of the rod.

compute_twist()
　　See *Knot Theory (Mixin)* for the detail.

compute_writhe(*type_of_additional_segment='next_tangent'*)
　　See *Knot Theory (Mixin)* for the detail.

Parameters

> **type_of_additional_segment** [str] Determines the method to compute new segments (elements) added to the rod. Valid inputs are "next_tangent", "end_to_end", "net_tangent", otherwise program uses the center line.

compute_link(*type_of_additional_segment='next_tangent'*)
> See *Knot Theory (Mixin)* for the detail.

Parameters

> **type_of_additional_segment** [str] Determines the method to compute new segments (elements) added to the rod. Valid inputs are "next_tangent", "end_to_end", "net_tangent", otherwise program uses the center line.

elastica.rod.knot_theory.compute_twist(*center_line*, *normal_collection*)
> Compute the twist of a rod, using center_line and normal collection.

> Methods used in this function is adapted from method 2a Klenin & Langowski 2000 paper.

> > **Warning:** If center line is straight, although the normals of each element is pointing different direction computed twist will be zero.

> Typical runtime of this function is longer than simulation steps. While we provide a function to compute topological quantities at every timesteps, **we highly recommend** to compute LWT during the post-processing stage.:

```python
import elastica
...
normal_collection = director_collection[:,0,...] # shape of director (time, 3, 3, n_
↪elems)
elastica.compute_twist(
    center_line,                              # shape (time, 3, n_nodes)
    normal_collection                         # shape (time, 3, n_elems)
)
```

Parameters

> **center_line** [numpy.ndarray] 3D (time, 3, n_nodes) array containing data with 'float' type. Time history of rod node positions.

> **normal_collection** [numpy.ndarray] 3D (time, 3, n_elems) array containing data with 'float' type. Time history of rod elements normal direction.

Returns

> **total_twist** [numpy.ndarray]

> **local_twist** [numpy.ndarray]

elastica.rod.knot_theory.compute_link(*center_line*, *normal_collection*, *radius*, *segment_length*, *type_of_additional_segment*)
> This function computes the total link history of a rod.

> Equations used are from method 1a from Klenin & Langowski 2000 paper.

> Typical runtime of this function is longer than simulation steps. While we provide a function to compute topological quantities at every timesteps, **we highly recommend** to compute LWT during the post-processing stage.:

```
import elastica
...
normal_collection = director_collection[:,0,...] # shape of director (time, 3, 3, n_
↪elems)
elastica.compute_link(
    center_line,                               # shape (time, 3, n_nodes)
    normal_collection,                         # shape (time 3, n_elems)
    radius,                                    # shape (time, n_elems)
    segment_length,
    type_of_additional_segment="next_tangent"
)
```

Parameters

> **center_line** [numpy.ndarray] 3D (time, 3, n_nodes) array containing data with 'float' type. Time history of rod node positions.
>
> **normal_collection** [numpy.ndarray] 3D (time, 3, n_elems) array containing data with 'float' type. Time history of rod elements normal direction.
>
> **radius** [numpy.ndarray] 2D (time, n_elems) array containing data with 'float' type. Time history of rod element radius.
>
> **segment_length** [float] Length of added segments.
>
> **type_of_additional_segment** [str] Determines the method to compute new segments (elements) added to the rod. Valid inputs are "next_tangent", "end_to_end", "net_tangent", otherwise program uses the center line.

Returns

> **total_link** [numpy.ndarray]

elastica.rod.knot_theory.**compute_writhe**(*center_line*, *segment_length*, *type_of_additional_segment*)
This function computes the total writhe history of a rod.

Equations used are from method 1a from Klenin & Langowski 2000 paper.

Typical runtime of this function is longer than simulation steps. While we provide a function to compute topological quantities at every timesteps, **we highly recommend** to compute LWT during the post-processing stage.:

```
import elastica
...
elastica.compute_writhe(
    center_line,                               # shape (time, 3, n_nodes)
    segment_length,
    type_of_additional_segment="next_tangent"
)
```

Parameters

> **center_line** [numpy.ndarray] 3D (time, 3, n_nodes) array containing data with 'float' type. Time history of rod node positions.
>
> **segment_length** [float] Length of added segments.
>
> **type_of_additional_segment** [str] Determines the method to compute new segments (elements) added to the rod. Valid inputs are "next_tangent", "end_to_end", "net_tangent", otherwise program uses the center line.

Returns

total_writhe [numpy.ndarray]

3.9 Rigid Body

type	
Cylinder	
Sphere	

class elastica.rigidbody.rigid_body.**RigidBodyBase**
Base class for rigid body classes.

Notes

All rigid body class should inherit this base class.

compute_position_center_of_mass()
Return positional center of mass

compute_translational_energy()
Return translational energy

compute_rotational_energy()
Return rotational energy

class elastica.rigidbody.cylinder.**Cylinder**(*start*, *direction*, *normal*, *base_length*, *base_radius*, *density*)

class elastica.rigidbody.sphere.**Sphere**(*center*, *base_radius*, *density*)

3.10 Constraints

Built-in boundary condition implementationss

3.10.1 Description

Constraints are equivalent to displacement boundary condition.

Available Constraint

ConstraintBase	Base class for constraint and displacement boundary condition implementation.
FreeBC	Boundary condition template.
OneEndFixedBC	This boundary condition class fixes one end of the rod.
FixedConstraint	This boundary condition class fixes the specified node or orientations.
HelicalBucklingBC	This is the boundary condition class for Helical Buckling case in Gazzola et.

continues on next page

<div align="center">

Table 1 – continued from previous page

</div>

FreeRod	Deprecated 0.2.1: Same implementation as FreeBC
OneEndFixedRod	Deprecated 0.2.1: Same implementation as OneEnd-FixedBC

Compatibility

Constraint / Boundary Condition	Rod	Rigid Body
FreeBC		
OneEndFixedBC		
FixedConstraint		
HelicalBucklingBC		

3.10.2 Examples

Note: PyElastica package provides basic built-in constraints, and we expect use to adapt their own boundary condition from our examples.

Customizing boundary condition examples:

- Flexible Swinging Pendulum

- Plectonemes

- Solenoids

3.10.3 Built-in Constraints

class elastica.boundary_conditions.**ConstraintBase**(*args*, ***kwargs*)

Bases: abc.ABC

Base class for constraint and displacement boundary condition implementation.

Notes

Constraint class must inherit BaseConstraint class.

> **Attributes**
>
>> *system* [RodBase or RigidBodyBase] get system (rod or rigid body) reference
>>
>> **node_indices** [None or numpy.ndarray]
>>
>> **element_indices** [None or numpy.ndarray]

property system: Union[Type[*elastica.rod.rod_base.RodBase*], Type[*elastica.rigidbody.rigid_body.RigidBodyBase*]]

get system (rod or rigid body) reference

> **Return type** Union[Type[*RodBase*], Type[*RigidBodyBase*]]

property constrained_position_idx: Optional[numpy.ndarray]

get position-indices passed to "using"

> **Return type** Optional[ndarray]

property constrained_director_idx: Optional[numpy.ndarray]
> get director-indices passed to "using"

> > **Return type** Optional[ndarray]

abstract constrain_values(*rod*, *time*)
> Constrain values (position and/or directors) of a rod object.

> > **Parameters**

> > > **rod** [Union[Type[RodBase], Type[RigidBodyBase]]] Rod or rigid-body object.

> > > **time** [float] The time of simulation.

> > > **:rtype:** [py:obj:*None*]

abstract constrain_rates(*rod*, *time*)
> Constrain rates (velocity and/or omega) of a rod object.

> > **Parameters**

> > > **rod** [Union[Type[RodBase], Type[RigidBodyBase]]] Rod or rigid-body object.

> > > **time** [float] The time of simulation.

> > > **:rtype:** [py:obj:*None*]

class elastica.boundary_conditions.FreeBC(***kwargs*)
> Boundary condition template.

class elastica.boundary_conditions.OneEndFixedBC(*fixed_position*, *fixed_directors*, ***kwargs*)
> This boundary condition class fixes one end of the rod. Currently, this boundary condition fixes position and directors at the first node and first element of the rod.

> Example case (timoshenko)

> **Examples**

> How to fix one ends of the rod:

> ```
> >>> simulator.constrain(rod).using(
> ...     OneEndFixedBC,
> ...     constrained_position_idx=(0,),
> ...     constrained_director_idx=(0,)
> ... )
> ```

> **__init__**(*fixed_position*, *fixed_directors*, ***kwargs*)
> > Initialization of the constraint. Any parameter passed to 'using' will be available in kwargs.

> > > **Parameters**

> > > > **constrained_position_idx** [tuple] Tuple of position-indices that will be constrained

> > > > **constrained_director_idx** [tuple] Tuple of director-indices that will be constrained

class elastica.boundary_conditions.FixedConstraint(**fixed_data*, ***kwargs*)
> This boundary condition class fixes the specified node or orientations. Index can be passed to fix either or both the position or the director. Constraining position is equivalent to setting 0 translational DOF. Constraining director is equivalent to setting 0 rotational DOF.

Examples

How to fix two ends of the rod:

```
>>> simulator.constrain(rod).using(
...     FixedConstraint,
...     constrained_position_idx=(0,1,-2,-1),
...     constrained_director_idx=(0,-1)
... )
```

How to pin the middle of the rod (10th node), without constraining the rotational DOF.

```
>>> simulator.constrain(rod).using(
...     FixedConstraint,
...     constrained_position_idx=(10)
... )
```

__init__(**fixed_data*, ***kwargs*)

> Initialization of the constraint. Any parameter passed to 'using' will be available in kwargs.

> > **Parameters**

> > > **constrained_position_idx** [tuple] Tuple of position-indices that will be constrained

> > > **constrained_director_idx** [tuple] Tuple of director-indices that will be constrained

class elastica.boundary_conditions.**HelicalBucklingBC**(*position_start*, *position_end*, *director_start*, *director_end*, *twisting_time*, *slack*, *number_of_rotations*, ***kwargs*)

This is the boundary condition class for Helical Buckling case in Gazzola et. al. RSoS (2018). The applied boundary condition is twist and slack on to the first and last nodes and elements of the rod.

Example case (helical buckling)

> **Attributes**

> > **twisting_time: float** Time to complete twist.

> > **final_start_position: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. Position of first node of rod after twist completed.

> > **final_end_position: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. Position of last node of rod after twist completed.

> > **ang_vel: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. Angular velocity of rod during twisting time.

> > **shrink_vel: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. Shrink velocity of rod during twisting time.

> > **final_start_directors: numpy.ndarray** 3D (dim, dim, 1) array containing data with 'float' type. Directors of first element of rod after twist completed.

> > **final_end_directors: numpy.ndarray** 3D (dim, dim, 1) array containing data with 'float' type. Directors of last element of rod after twist completed.

__init__(*position_start*, *position_end*, *director_start*, *director_end*, *twisting_time*, *slack*, *number_of_rotations*, ***kwargs*)

> Helical Buckling initializer

> > **Parameters**

> > **position_start** [numpy.ndarray] 2D (dim, 1) array containing data with 'float' type. Initial position of first node.
>
> > **position_end** [numpy.ndarray] 2D (dim, 1) array containing data with 'float' type. Initial position of last node.
>
> > **director_start** [numpy.ndarray] 3D (dim, dim, blocksize) array containing data with 'float' type. Initial director of first element.
>
> > **director_end** [numpy.ndarray] 3D (dim, dim, blocksize) array containing data with 'float' type. Initial director of last element.
>
> > **twisting_time** [float] Time to complete twist.
>
> > **slack** [float] Slack applied to rod.
>
> > **number_of_rotations** [float] Number of rotations applied to rod.

class elastica.boundary_conditions.**FreeRod**(***kwargs*)

> Deprecated 0.2.1: Same implementation as FreeBC

class elastica.boundary_conditions.**OneEndFixedRod**(*fixed_position*, *fixed_directors*, ***kwargs*)

> Deprecated 0.2.1: Same implementation as OneEndFixedBC

3.11 External Forces / Interactions

3.11.1 Description

External force and environmental interaction are represented as force/torque boundary condition at different location.

Available Forcing

Numba implementation module for boundary condition implementations that apply external forces to the rod.

NoForces	This is the base class for external forcing boundary conditions applied to rod-like objects.
EndpointForces	This class applies constant forces on the endpoint nodes.
GravityForces	This class applies a constant gravitational force to the entire rod.
UniformForces	This class applies a uniform force to the entire rod.
UniformTorques	This class applies a uniform torque to the entire rod.
MuscleTorques	This class applies muscle torques along the body.

Available Interaction

Numba implementation module containing interactions between a rod and its environment.

AnisotropicFrictionalPlane	This anisotropic friction plane class is for computing anisotropic friction forces on rods.
InteractionPlane	The interaction plane class computes the plane reaction force on a rod-like object.

Table 3 – continued from previous page

SlenderBodyTheory	This slender body theory class is for flow-structure interaction problems.

Compatibility

Forcing	Rod	Rigid Body
NoForces		
EndpointForces		
GravityForces		
UniformForces		
UniformTorques		
MuscleTorques		

Interaction	Rod	Rigid Body
AnisotropicFrictionalPlane		
InteractionPlane		
SlenderBodyTheory		

3.11.2 Built-in External Forces

Numba implementation module for boundary condition implementations that apply external forces to the rod.

class elastica.external_forces.**NoForces**

This is the base class for external forcing boundary conditions applied to rod-like objects.

Notes

Every new external forcing class must be derived from NoForces class.

__init__()

NoForces class does not need any input parameters.

class elastica.external_forces.**EndpointForces**(*start_force*, *end_force*, *ramp_up_time=0.0*)

This class applies constant forces on the endpoint nodes.

Attributes

start_force: numpy.ndarray 2D (dim, 1) array containing data with 'float' type. Force applied to first node of the rod-like object.

end_force: numpy.ndarray 2D (dim, 1) array containing data with 'float' type. Force applied to last node of the rod-like object.

ramp_up_time: float Applied forces are ramped up until ramp up time.

__init__(*start_force*, *end_force*, *ramp_up_time=0.0*)

Parameters

start_force: numpy.ndarray 2D (dim, 1) array containing data with 'float' type. Force applied to first node of the rod-like object.

end_force: numpy.ndarray 2D (dim, 1) array containing data with 'float' type. Force applied to last node of the rod-like object.

ramp_up_time: float Applied forces are ramped up until ramp up time.

class elastica.external_forces.**GravityForces**(*acc_gravity=array([0.0, - 9.80665, 0.0])*)
This class applies a constant gravitational force to the entire rod.

Attributes

acc_gravity: numpy.ndarray 1D (dim) array containing data with 'float' type. Gravitational acceleration vector.

__init__(*acc_gravity=array([0.0, - 9.80665, 0.0])*)

Parameters

acc_gravity: numpy.ndarray 1D (dim) array containing data with 'float' type. Gravitational acceleration vector.

class elastica.external_forces.**UniformForces**(*force*, *direction=array([0.0, 0.0, 0.0])*)
This class applies a uniform force to the entire rod.

Attributes

force: numpy.ndarray 2D (dim, 1) array containing data with 'float' type. Total force applied to a rod-like object.

__init__(*force*, *direction=array([0.0, 0.0, 0.0])*)

Parameters

force: float Force magnitude applied to a rod-like object.

direction: numpy.ndarray 1D (dim) array containing data with 'float' type. Direction in which force applied.

class elastica.external_forces.**UniformTorques**(*torque*, *direction=array([0.0, 0.0, 0.0])*)
This class applies a uniform torque to the entire rod.

Attributes

torque: numpy.ndarray 2D (dim, 1) array containing data with 'float' type. Total torque applied to a rod-like object.

__init__(*torque*, *direction=array([0.0, 0.0, 0.0])*)

Parameters

torque: float Torque magnitude applied to a rod-like object.

direction: numpy.ndarray 1D (dim) array containing data with 'float' type. Direction in which torque applied.

class elastica.external_forces.**MuscleTorques**(*base_length*, *b_coeff*, *period*, *wave_number*, *phase_shift*, *direction*, *rest_lengths*, *ramp_up_time=0.0*, *with_spline=False*)
This class applies muscle torques along the body. The applied muscle torques are treated as applied external forces. This class can apply muscle torques as a traveling wave with a beta spline or only as a traveling wave. For implementation details refer to Gazzola et. al. RSoS. (2018).

Attributes

direction: numpy.ndarray 2D (dim, 1) array containing data with 'float' type. Muscle torque direction.

angular_frequency: float Angular frequency of traveling wave.

wave_number: float Wave number of traveling wave.

phase_shift: float Phase shift of traveling wave.

ramp_up_time: float Applied muscle torques are ramped up until ramp up time.

my_spline: numpy.ndarray 1D (blocksize) array containing data with 'float' type. Generated spline.

__init__(*base_length*, *b_coeff*, *period*, *wave_number*, *phase_shift*, *direction*, *rest_lengths*, *ramp_up_time=0.0*, *with_spline=False*)

Parameters

base_length: float Rest length of the rod-like object.

b_coeff: nump.ndarray 1D array containing data with 'float' type. Beta coefficients for beta-spline.

period: float Period of traveling wave.

wave_number: float Wave number of traveling wave.

phase_shift: float Phase shift of traveling wave.

direction: numpy.ndarray 1D (dim) array containing data with 'float' type. Muscle torque direction.

ramp_up_time: float Applied muscle torques are ramped up until ramp up time.

with_spline: boolean Option to use beta-spline.

3.11.3 Built-in Environment Interactions

Numba implementation module containing interactions between a rod and its environment.

class elastica.interaction.**AnisotropicFrictionalPlane**(*k*, *nu*, *plane_origin*, *plane_normal*, *slip_velocity_tol*, *static_mu_array*, *kinetic_mu_array*)

This anisotropic friction plane class is for computing anisotropic friction forces on rods. A detailed explanation of the implemented equations can be found in Gazzola et al. RSoS. (2018).

Attributes

k: float Stiffness coefficient between the plane and the rod-like object.

nu: float Dissipation coefficient between the plane and the rod-like object.

plane_origin: numpy.ndarray 2D (dim, 1) array containing data with 'float' type. Origin of the plane.

plane_normal: numpy.ndarray 2D (dim, 1) array containing data with 'float' type. The normal vector of the plane.

slip_velocity_tol: float Velocity tolerance to determine if the element is slipping or not.

static_mu_array: numpy.ndarray 1D (3,) array containing data with 'float' type. [forward, backward, sideways] static friction coefficients.

> > **kinetic_mu_array: numpy.ndarray** 1D (3,) array containing data with 'float' type. [forward, backward, sideways] kinetic friction coefficients.

> **__init__**(*k*, *nu*, *plane_origin*, *plane_normal*, *slip_velocity_tol*, *static_mu_array*, *kinetic_mu_array*)

> > **Parameters**

> > > **k: float** Stiffness coefficient between the plane and the rod-like object.

> > > **nu: float** Dissipation coefficient between the plane and the rod-like object.

> > > **plane_origin: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. Origin of the plane.

> > > **plane_normal: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. The normal vector of the plane.

> > > **slip_velocity_tol: float** Velocity tolerance to determine if the element is slipping or not.

> > > **static_mu_array: numpy.ndarray** 1D (3,) array containing data with 'float' type. [forward, backward, sideways] static friction coefficients.

> > > **kinetic_mu_array: numpy.ndarray** 1D (3,) array containing data with 'float' type. [forward, backward, sideways] kinetic friction coefficients.

class elastica.interaction.**InteractionPlane**(*k*, *nu*, *plane_origin*, *plane_normal*)

> The interaction plane class computes the plane reaction force on a rod-like object. For more details regarding the contact module refer to Eqn 4.8 of Gazzola et al. RSoS (2018).

> > **Attributes**

> > > **k: float** Stiffness coefficient between the plane and the rod-like object.

> > > **nu: float** Dissipation coefficient between the plane and the rod-like object.

> > > **plane_origin: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. Origin of the plane.

> > > **plane_normal: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. The normal vector of the plane.

> > > **surface_tol: float** Penetration tolerance between the plane and the rod-like object.

> **__init__**(*k*, *nu*, *plane_origin*, *plane_normal*)

> > **Parameters**

> > > **k: float** Stiffness coefficient between the plane and the rod-like object.

> > > **nu: float** Dissipation coefficient between the plane and the rod-like object.

> > > **plane_origin: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. Origin of the plane.

> > > **plane_normal: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. The normal vector of the plane.

class elastica.interaction.**SlenderBodyTheory**(*dynamic_viscosity*)

> This slender body theory class is for flow-structure interaction problems. This class applies hydrodynamic forces on the body using the slender body theory given in Eq. 4.13 of Gazzola et al. RSoS (2018).

> > **Attributes**

> > > **dynamic_viscosity: float** Dynamic viscosity of the fluid.

__init__(*dynamic_viscosity*)

> **Parameters**
>
> > **dynamic_viscosity** [float] Dynamic viscosity of the fluid.

3.12 Connections / Contact / Joints

Module containing joint classes to connect multiple rods together.

3.12.1 Description

Available Connection/Contact/Joints

FreeJoint	This free joint class is the base class for all joints.
ExternalContact	Assumes that the second entity is a rigid body for now, can be changed at a later time
FixedJoint	The fixed joint class restricts the relative movement and rotation between two nodes and elements by applying restoring forces and torques.
HingeJoint	This hinge joint class constrains the relative movement and rotation (only one axis defined by the user) between two nodes and elements (chosen by the user) by applying restoring forces and torques.
SelfContact	This class is modeling self contact of rod.

Compatibility

Connection / Contact / Joints	Rod	Rigid Body
FreeJoint		
ExternalContact		
FixedJoint		
HingeJoint		
SelfContact		

3.12.2 Built-in Connection / Contact / Joint

class elastica.joint.**FreeJoint**(*k*, *nu*)

This free joint class is the base class for all joints. Free or spherical joints constrains the relative movement between two nodes (chosen by the user) by applying restoring forces. For implementation details, refer to Zhang et al. Nature Communications (2019).

Notes

Every new joint class must be derived from the FreeJoint class.

Attributes

k: float Stiffness coefficient of the joint.

nu: float Damping coefficient of the joint.

__init__(*k*, *nu*)

Parameters

k: float Stiffness coefficient of the joint.

nu: float Damping coefficient of the joint.

class elastica.joint.**ExternalContact**(*k*, *nu*)

Assumes that the second entity is a rigid body for now, can be changed at a later time

Most of the cylinder-cylinder contact SHOULD be implemented as given in this paper.

but, it isn't (the elastica-cpp kernels are implented)! This is maybe to speed-up the kernel, but it's potentially dangerous as it does not deal with "end" conditions correctly.

__init__(*k*, *nu*)

Parameters

k: float Stiffness coefficient of the joint.

nu: float Damping coefficient of the joint.

class elastica.joint.**FixedJoint**(*k*, *nu*, *kt*)

The fixed joint class restricts the relative movement and rotation between two nodes and elements by applying restoring forces and torques. For implementation details, refer to Zhang et al. Nature Communications (2019).

Attributes

k: float Stiffness coefficient of the joint.

nu: float Damping coefficient of the joint.

kt: float Rotational stiffness coefficient of the joint.

__init__(*k*, *nu*, *kt*)

Parameters

k: float Stiffness coefficient of the joint.

nu: float Damping coefficient of the joint.

kt: float Rotational stiffness coefficient of the joint.

class `elastica.joint.`**HingeJoint**(*k*, *nu*, *kt*, *normal_direction*)

> This hinge joint class constrains the relative movement and rotation (only one axis defined by the user) between two nodes and elements (chosen by the user) by applying restoring forces and torques. For implementation details, refer to Zhang et. al. Nature Communications (2019).
>
> > **Attributes**
> >
> > > **k: float** Stiffness coefficient of the joint.
> > >
> > > **nu: float** Damping coefficient of the joint.
> > >
> > > **kt: float** Rotational stiffness coefficient of the joint.
> > >
> > > **normal_direction: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. Constraint rotation direction.
>
> **__init__**(*k*, *nu*, *kt*, *normal_direction*)
>
> > **Parameters**
> >
> > > **k: float** Stiffness coefficient of the joint.
> > >
> > > **nu: float** Damping coefficient of the joint.
> > >
> > > **kt: float** Rotational stiffness coefficient of the joint.
> > >
> > > **normal_direction: numpy.ndarray** 2D (dim, 1) array containing data with 'float' type. Constraint rotation direction.

class `elastica.joint.`**SelfContact**(*k*, *nu*)

> This class is modeling self contact of rod.
>
> **__init__**(*k*, *nu*)
>
> > **Parameters**
> >
> > > **k: float** Stiffness coefficient of the joint.
> > >
> > > **nu: float** Damping coefficient of the joint.

3.13 Callback Functions

Module contains callback classes to save simulation data for rod-like objects

3.13.1 Description

The frequency at which you have your callback function save data will depend on what information you need from the simulation. Excessive call backs can cause performance penalties, however, it is rarely necessary to make call backs at a frequency that this becomes a problem. We have found that making a call back roughly every 100 iterations has a negligible performance penalty.

Currently, all data saved from call back functions is saved in memory. If you have many rods or are running for a long time, you may want to consider editing the call back function to write the saved data to disk so you do not run out of memory during the simulation.

CallBackBaseClass	This is the base class for callbacks for rod-like objects.

3.13.2 Built-in Constraints

class elastica.callback_functions.**CallBackBaseClass**
    This is the base class for callbacks for rod-like objects.

Notes

Every new callback class must be derived from CallBackBaseClass.

    __init__()
        CallBackBaseClass does not need any input parameters.

class elastica.callback_functions.**ExportCallBack**(*step_skip*, *path*, *method*, *initial_file_count=0*,
                                                    save_every=100000000.0)
    ExportCallback is an example callback class to demonstrate how to export rod-data into data file.

    If one wants to customize the saving data, we recommend to override *make_callback* method.

        Attributes

            AVAILABLE_METHOD Supported method to save the file. We recommend binary save to
                maintain the tensor structure of data.

            FILE_SIZE_CUTOFF Maximum buffer size for each file. If the buffer size exceed, new file is
                created. Actual size of the file is expected to be marginally larger.

    __init__(*step_skip*, *path*, *method*, *initial_file_count=0*, *save_every=100000000.0*)

        Parameters

            step_skip [int] Collect data at each step_skip steps.

            path [str] Path to save the file. If directories are prepended, they must exist. The filename
                depends on the method. The path is not expected to include extension.

            method [str] Method name. Only the name in AVAILABLE_METHOD is allowed.

            initial_file_count [int] Initial file count index that will be appended

            save_every [int] Save the file every save_every steps. (default=1e8)

class elastica.callback_functions.**MyCallBack**(*step_skip*, *callback_params*)
    MyCallBack class is derived from the base callback class. This is just an example of a callback class, this class
    as an example/template to write new call back classes in your client file.

        Attributes

            sample_every: int Collect data using make_callback method every sampling step.

            callback_params: dict Collected callback data is saved in this dictionary.

    __init__(*step_skip*, *callback_params*)

        Parameters

> **step_skip: int** Collect data using make_callback method every step_skip step.
>
> **callback_params: dict** Collected data is saved in this dictionary.

3.14 Time steppers

Symplectic time steppers and concepts for integrating the kinematic and dynamic equations of rod-like objects.

class `elastica.timestepper.symplectic_steppers.`**`PositionVerlet`**
> Position Verlet symplectic time stepper class, which includes methods for second-order position Verlet.

class `elastica.timestepper.symplectic_steppers.`**`PEFRL`**
> Position Extended Forest-Ruth Like Algorithm of I.M. Omelyan, I.M. Mryglod and R. Folk, Computer Physics Communications 146, 188 (2002), http://arxiv.org/abs/cond-mat/0110585

3.15 Simulator

3.15.1 Base System

Basic coordinating for multiple, smaller systems that have an independently integrable interface (i.e. works with symplectic or explicit routines *timestepper.py*.)

class `elastica.wrappers.base_system.`**`BaseSystemCollection`**
> Base System for simulator classes. Every simulation class written by the user must be derived from the BaseSystemCollection class; otherwise the simulation will proceed.
>
> > **Attributes**
> >
> > > **allowed_sys_types: tuple** Tuple of allowed type rod-like objects. Here use a base class for objects, i.e. RodBase.
> > >
> > > **_systems: list** List of rod-like objects.
>
> **`finalize`**`()`
> > This method finalizes the simulator class. When it is called, it is assumed that the user has appended all rod-like objects to the simulator as well as all boundary conditions, callbacks, etc., acting on these rod-like objects. After the finalize method called, the user cannot add new features to the simulator class.

3.15.2 CallBacks

Provides the callBack interface to collect data over time (see *callback_functions.py*).

class `elastica.wrappers.callbacks.`**`CallBacks`**
> CallBacks class is a wrapper for calling callback functions, set by the user. If the user wants to collect data from the simulation, the simulator class has to be derived from the CallBacks class.
>
> > **Attributes**
> >
> > > **_callback_list: list** List of call back classes defined for rod-like objects.
>
> **`collect_diagnostics`**`(`*system*`)`
> > This method calls user-defined call-back classes for a user-defined system or rod-like object. You need to input the system or rod-like object that you want to collect data from.
> >
> > > **Parameters**

> **system: object** System is a rod-like object.

> **Returns**

3.15.3 Connect

Provides the connections interface to connect entities (rods, rigid bodies) using joints (see *joints.py*).

class elastica.wrappers.connections.**Connections**
> The Connections class is a wrapper for connecting rod-like objects using joints selected by the user. To connect two rod-like objects, the simulator class must be derived from the Connections class.

> > **Attributes**

> > > **_connections: list** List of joint classes defined for rod-like objects.

connect(*first_rod*, *second_rod*, *first_connect_idx=None*, *second_connect_idx=None*)
> This method connects two rod-like objects using the selected joint class. You need to input the two rod-like objects that are to be connected as well as set the element indexes of these rods where the connection occurs.

> > **Parameters**

> > > **first_rod** [object] Rod-like object

> > > **second_rod** [object] Rod-like object

> > > **first_connect_idx** [int] Index of first rod for joint.

> > > **second_connect_idx** [int] Index of second rod for joint.

> > **Returns**

3.15.4 Constraints

Provides the constraints interface to enforce displacement boundary conditions (see *boundary_conditions.py*).

class elastica.wrappers.constraints.**Constraints**
> The Constraints class is a wrapper for enforcing displacement boundary conditions. To enforce boundary conditions on rod-like objects, the simulator class must be derived from Constraints class.

> > **Attributes**

> > > **_constraints: list** List of boundary condition classes defined for rod-like objects.

constrain(*system*)
> This method enforces a displacement boundary conditions to the relevant user-defined system or rod-like object. You must input the system or rod-like object that you want to enforce boundary condition on.

> > **Parameters**

> > > **system: object** System is a rod-like object.

> > **Returns**

3.15.5 Forcing

Provides the forcing interface to apply forces and torques to rod-like objects (external point force, muscle torques, etc).

class elastica.wrappers.forcing.**Forcing**
> The Forcing class is a wrapper for applying boundary conditions that consist of applied external forces. To apply forcing on rod-like objects, the simulator class must be derived from the Forcing class.
>
> > **Attributes**
> >
> > > **_ext_forces_torques: list** List of forcing class defined for rod-like objects.
>
> add_forcing_to(*system*)
> > This method applies external forces and torques on the relevant user-defined system or rod-like object. You must input the system or rod-like object that you want to apply external forces and torques on.
> >
> > > **Parameters**
> > >
> > > > **system: object** System is a rod-like object.
> > >
> > > **Returns**

3.16 Utility Functions

Here, we provide some useful functions that we often use along with elastica.

3.16.1 Transformations

Rotation interface functions

elastica.transformations.**inv_skew_symmetrize**(*matrix_collection*)
> Safe wrapper around inv_skew_symmetrize that does checking and formatting on type of matrix_collection using format_matrix_shape function.
>
> > **Parameters**
> >
> > > **matrix_collection: numpy.ndarray**
> >
> > **Returns**

elastica.transformations.**rotate**(*matrix*, *scale*, *axis*)
> This function takes single or multiple frames as matrix. Then rotates these frames around a single axis for all frames, or can rotate each frame around its own rotation axis as defined by user. Scale determines how much frames rotates around this axis.
>
> matrix: minimum shape = dim**2x1, supports shape = 3x3xn axis: minimum dim = 3x1, 1x3, supports dim = 3xn, nx3 scale: minimum float, supports 1D vectors also dim = n

3.16.2 Math

Quadrature and difference kernels

elastica._calculus.**position_difference_kernel**(*vector*)

This function computes difference between elements of a batch vector.

> **Parameters**
>
> > **vector: numpy.ndarray** 2D (dim, blocksize) array containing data with 'float' type.
>
> **Returns**
>
> > **result: numpy.ndarray** 2D (dim, blocksize-1) array containing data with 'float' type.

> ### Notes
>
> Micro benchmark results showed that for a block size of 100, using timeit Python version: 3.29 µs ± 767 ns per loop This version: 840 ns ± 14.5 ns per loop

elastica._calculus.**position_average**(*vector*)

This function computes the average between elements of a vector.

> **Parameters**
>
> > **vector** [numpy.ndarray] 1D (blocksize) array containing data with 'float' type.
>
> **Returns**
>
> > **result: numpy.ndarray** 1D (blocksize-1) array containing data with 'float' type.

> ### Notes
>
> Micro benchmark results showed that for a block size of 100, using timeit Python version: 2.37 µs ± 764 ns per loop This version: 713 ns ± 3.69 ns per loop

elastica._calculus.**quadrature_kernel**(*array_collection*)

Simple trapezoidal quadrature rule with zero at end-points, in a dimension agnostic way

> **Parameters**
>
> > **array_collection** [numpy.ndarray] 2D (dim, blocksize) array containing data with 'float' type.
>
> **Returns**
>
> > **result: numpy.ndarray** 2D (dim, blocksize+1) array containing data with 'float' type.

> ### Notes
>
> Micro benchmark results, for a block size of 100, using timeit Python version: 8.14 µs ± 1.42 µs per loop This version: 781 ns ± 18.3 ns per loop

elastica._calculus.**difference_kernel**(*array_collection*)

This function does differentiation.

> **Parameters**
>
> > **array_collection** [numpy.ndarray] 2D (dim, blocksize) array containing data with 'float' type.
>
> **Returns**
>
> > **result: numpy.ndarray** 2D (dim, blocksize-1) array containing data with 'float' type.

Notes

Micro benchmark results showed that for a block size of 100, using timeit Python version: 9.07 µs $\pm$ 2.15 µs per loop This version: 952 ns $\pm$ 91.1 ns per loop

elastica._calculus.**quadrature_kernel_for_block_structure**(*array_collection*, *ghost_idx*)
    Simple trapezoidal quadrature rule with zero at end-points, in a dimension agnostic way. This form specifically for the block structure implementation and there is a reset function call, to reset ghosts.

> **Parameters**
>
> > **array_collection** [numpy.ndarray] 2D (dim, blocksize) array containing data with 'float' type.
> >
> > **ghost_idx** [numpy.ndarray] 1D (n_ghost) array containing data with 'int' type.
>
> **Returns**
>
> > **result: numpy.ndarray** 2D (dim, blocksize+1) array containing data with 'float' type.

> ### Notes
>
> Micro benchmark results, for a block size of 100, using timeit Python version: 8.21 µs per loop This version: 1.03 µs per loop
>
> User should use this function with extreme care, since this function is rewritten for block structure.

elastica._calculus.**difference_kernel_for_block_structure**(*array_collection*, *ghost_idx*)
    This function does the differentiation, for Cosserat rod model equations. This form specifically for the block structure implementation and there is a reset function call, to reset ghosts.

> **Parameters**
>
> > **array_collection** [numpy.ndarray] 2D (dim, blocksize) array containing data with 'float' type.
> >
> > **ghost_idx** [numpy.ndarray] 1D (n_ghost) array containing data with 'int' type.
>
> **Returns**
>
> > **result: numpy.ndarray** 2D (dim, blocksize-1) array containing data with 'float' type.

> ### Notes
>
> Micro benchmark results showed that for a block size of 100, using timeit Python version: 7.1 µs per loop This version: 1.01 µs per loop
>
> User should use this function with extreme care, since this function is rewritten for block structure.

Convenient linear algebra kernels

elastica._linalg.**levi_civita_tensor**(*dim*)

> > **Parameters**
> >
> > > **dim**
> >
> > **Returns**

Rotation kernels

3.16.3 Miscellaneous

Handy utilities

elastica.utils.**isqrt**(*num*)

> Efficiently computes sqrt for integer values

> Dropin replacement for python3.8's isqrt function Credits : https://stackoverflow.com/a/53983683

> > **Parameters**
> >
> > > **num** [int, input]
> >
> > **Returns**
> >
> > > **sqrt_num** [int, rounded down sqrt of num]

> **Notes**

> - Doesn't handle edge-cases of negative numbers by design
> - Doesn't type-check for integers by design, although it is hinted at

> **Examples**

> > **Return type** int

3.17 Localized Force and Torque

> Originated by the investigation in the issue #39

3.17.1 Discussion

In elastica, **a force is applied on a node** while **a torque is applied on an element**. For example, a localized force EndpointForce is applied only on a node. However, we found that adding additional torque on a neighboring elements, such that the torque represent a local moment induced by the point-force, could yield better convergence. We haven't found any evidence (yet) that this actually changes the steady-state configuration and kinematics, since it is two different implementation of the same point-load. We suspect the improvement by adding additional torque is due to explicitly giving the force-boundary condition that match the final internal-stress state.

3.17.2 Comparison

Factoring the additional-torque on a neighboring element leads to slightly better error estimates for the Timoshenko beam example. The results are condensed here. With new implementation, we achieved the same error with less number of discretization, but it also requires additional torque computation.

3.17.3 Modified Implementation

```python
class EndpointForcesWithTorques(NoForces):
    """
    This class applies constant forces on the endpoint nodes.
    """

    def __init__(self, end_force, ramp_up_time=0.0):
        """

        Parameters
        ----------
        start_force: numpy.ndarray
            2D (dim, 1) array containing data with 'float' type.
            Force applied to first node of the rod-like object.
        end_force: numpy.ndarray
            2D (dim, 1) array containing data with 'float' type.
            Force applied to last node of the rod-like object.
        ramp_up_time: float
            Applied forces are ramped up until ramp up time.

        """
        self.end_force = end_force
        assert ramp_up_time >= 0.0
        self.ramp_up_time = ramp_up_time

    def apply_forces(self, system, time=0.0):
        factor = min(1.0, time / self.ramp_up_time)
        self.external_forces[..., -1] += self.end_force * factor

    def apply_torques(self, system, time: np.float64 = 0.0):
        factor = min(1.0, time / self.ramp_up_time)
        arm_length = system.lengths[...,-1]
        director = system.director_collection[..., -1]
        self.external_torques[..., -1] += np.cross(
            [0.0, 0.0, 0.5 * arm_length], director @ self.end_force
        )
```

3.18 Code Design: Mixin and Composition

Elastica package follows Mixin and composition design patterns that may be unfamiliar to users. Here is a collection of references that introduce the package design.

3.18.1 References

- stackoverflow discussion on Mixin
- example of Mixin: python collections

3.19 Hackathon Readme

NCSA-NVIDIA AI Hackathon held at the University of Illinois from March 7-8 2020.

3.19.1 Problem Statement

The objective is to train a model to move a (cyber)-octopus with two soft arms and a head to reach a target location, and then grab an object. The octopus is modeled as an assembly of Cosserat rods and is activated by muscles surrounding its arms. Input to the mechanical model is the activation signals to the surrounding muscles, which causes it to contract, thus moving the arms. The output of the model comes from the octopus' environment. The mechanical model will be provided both for the octopus and its interaction with its environment. The goal is to find the correct muscle activation signals that make the octopus crawl to reach the target location and then make one arm to grab the object.

3.19.2 Progression of specific goals

These goals build on each other, you need to successfully accomplish all prior goals to get credit for later goals.

1) Make octopus crawl towards some direction. (5 points)

2) Make your octopus crawl to the target location. (7.5 points)

3) Make octopus to move the object using its arms. (7.5 points)

4) Have your octopus grab the object by wrapping one arm around the object. (10 points)

5) Make your octopus return to its starting location with the object. (20 points)

6) Generalize your policy to perform these tasks for an arbitrarily located object. (50 points)

3.19.3 Problem Context

Octopuses have flexible limbs made up of muscles with no internal bone structure. These limbs, know as muscular hydrostats, have an almost infinite number of degrees of freedom, allowing an octopus to perform complex actions with its arms, but also making them difficult to mathematically model. Attempts to model octopus arms are motivated not only by a desire to understand them biologically, but also to adapt their control ability and decision making processes to the rapidly developing field of soft robotics. We have developed a simulation package Elastica that models flexible 1-d rods, which can be used to represent octopus arms as a long, slender rod. We now want to learn methods for controlling these arms.

You are being provided with a model of an octopus that consists of two arms connected by a head. Each arm can be controlled independently. These arms are actuated through the contraction of muscles in the arms. This muscle activation produces a torque profile along the arm, resulting in movement of the arm. The arms interact with the ground through friction. Your goal is to teach the octopus to crawl towards an object, grab it, and bring it back to where the octopus started.

3.19.4 Controlling octopus arms with hierarchical basis functions

For this problem, we abstract the activation of the octopus muscles to the generation of a torque profile defined by the activation of a set of hierarchical radial basis function. Here we are using Gaussian basis functions.
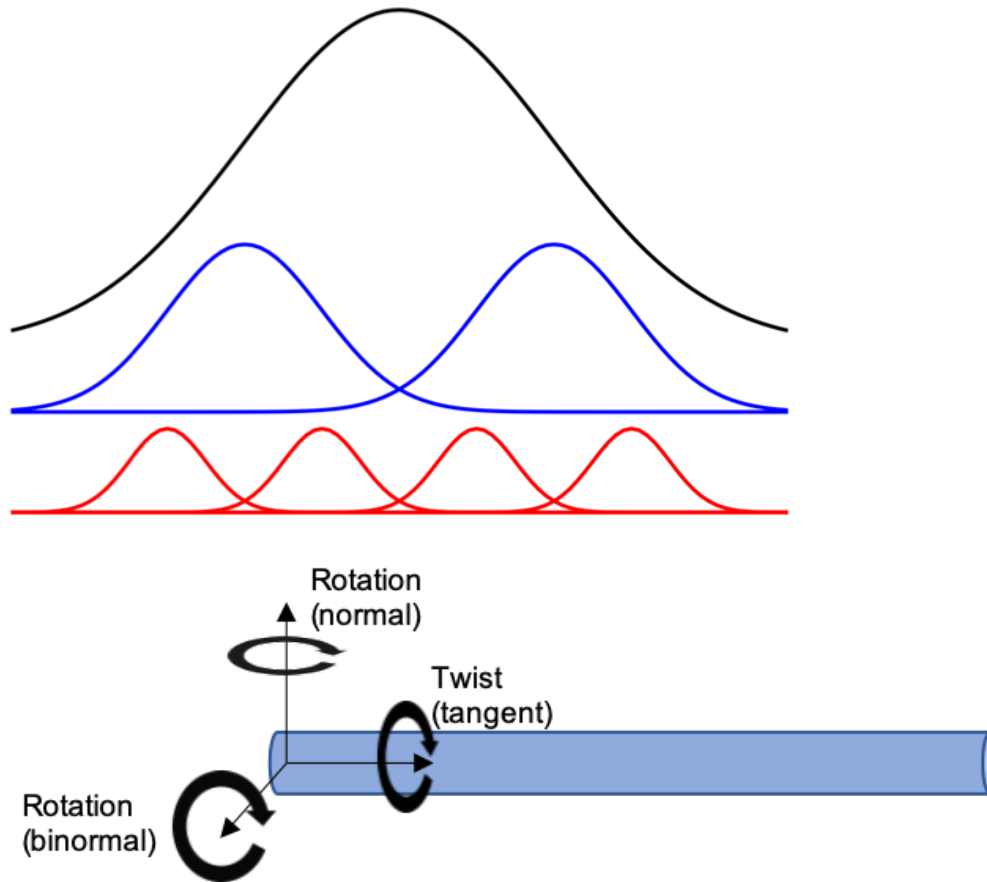
There are three levels of these basis functions, with 1 basis function in the first level, 2 in the second level and 4 in the third, leading to 7 basis functions in set. These levels have different maximum levels of activation. The lower levels have larger magnitudes than the higher levels, meaning they represent bulk motion of the rod while the higher levels allow finer control of the rod along the interval. In the code, the magnitude of each level will be fixed but you can choose the amount of activation at each level by setting the activation level between -1 and 1.

There are two bending modes (in the normal and binormal directions) and a twisting mode (in the tangent direction), so we define torques in these three different directions and independently for each arm. This yields six different sets of basis functions that can be activated for a total of 42 inputs.

3.19.5 Overview of provided Elastica code

We are providing you the Elastica software package which is written in Python. Elastica simulates the dynamics and kinematics of 1-d slender rods. We have set up the model for you such that you do not need to worry about the details of the model, only the activation patterns of the muscle. In the provided `examples/ArmWithBasisFunctions/two_arm_octopus_ai_imp.py` file you will import the `Environment` class which will define and setup the simulation.

`Environment` has three relevant functions:

- `Environment.reset(self)`: setups and initializes the simulation environment. Call this prior to running any simulations.

- `Environment.step(self, activation_array_list, time)`: takes one timestep for muscle activations defined in `activation_array_list`.

- `Environment.post_processing(self, filename_video)`: Makes 3D video based on saved data from simulation. Requires `ffmpeg`.
  We do not suggest changing `Environment` as it may cause unintended consequences to the simulation.

You will want to work within `main()` to interface with the simulations and develop your learning model. In `main()`, the first thing you need to define is the length of your simulation and initialize the environment. `final_time` is the length of time that your simulation will run unless exited early. You want to give your octopus enough time to complete the task, but too much time will lead to excessively long simulation times.

```python
# Set simulation final time
final_time = 10.0

# Initialize the environment
target_position = np.array([-0.4, 0.0, 0.5])
env = Environment(final_time, target_position, COLLECT_DATA_FOR_POSTPROCESSING=True)
total_steps, systems = env.reset()
```

With your system initialized, you are now ready to perform the simulation. To perform the simulation there are two steps:

1) Evaluate the reward function and define the basis function activations

2) Perform time step

There is also a user defined stopping condition. When met, this will immediately end the simulation. This can be useful to end the simulation if the octopus successfully complete the task early, or has a sufficiently low reward function that there is no point continuing the simulation.

```python
for i_sim in tqdm(range(total_steps)):
    """ Learning loop """
    if i_sim % 200:
        """ Add your learning algorithm here to define activation """
        # This will be based on your observations of the system and
        # evaluation of your reward function.
        shearable_rod = systems[0]
        rigid_body = systems[1]
        reward = reward_function()
        activation = segment_activation_function()

    """ Perform time step """
    time, systems, done = env.step(activation, time)

    """ User defined condition to exit simulation loop """
    done = user_defined_condition_function(reward, systems, time)
    if done:
        break
```

The state of the octopus is available in `shearable_rod`. The octopus consists of a series of 121 nodes. Nodes 0-49 relate to one arm, nodes 50-70 relate to the head, and nodes 71-120 relate to the second arm. `shearable_rod.position_collection` returns an array with entries relating to the position of each node. The state of the target object is available in `rigid_body`.

It is important to properly define the activation function. It consists of a list of lists defining the activation of the two arms in each of the the three modes of deformation. The activation function should be a list with three entries for the three modes of deformation. Each of these entries is in turn a list with two entries, which are arrays of the basis function activations for the two arms.

```
activation = [
    [arm_1_normal,   arm_2_normal],    # activation in normal direction
    [arm_1_binormal, arm_2_binormal],  # activation in binormal direction
    [arm_1_tangent,  arm_2_tangent],   # activation in tangent direction
    ]
```

Each activation array has 7 entries that relate to the activation of different basis functions. The ordering goes from the top level to the bottom level of the hierarchy. Each entry can vary from -1 to 1.

`activation_array[0]` – One top level muscle segment
`activation_array[1:3]` – Two mid level muscle segment
`activation_array[3:7]` – Four bottom level muscle segment

3.19.6 A few practical notes

1) To save a video of the octopus with `Environment.post_processing()`, you need to install `ffmeg`. You can download and install it here.

2) The timestep size is set to 40 s. This is necessary to keep the simulation stable, however, you may not need to update your muscle activations that often. Varying the learning time step will change how often your octopus updates its behaviour.

3) There is a 15-20 second startup delay while the simulation is initialized. This is a one time cost whenever the Python script is run and resetting the simulation using `.rest()` does not incur this delay for subsequent simulations.

4) We suggest installing `requirements.txt` and `optional-requirements.txt`, to run Elastica without any problem.

3.20 Indices and tables

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PYTHON MODULE INDEX

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