Parampool Tutorial

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Abstract

Parampool is a Python package for handling a potentially large pool of input parameters in scientific applications. The simplest use is to pass a Python function to Parampool and get back a web interface for setting the arguments to the function. More powerful use consists in defining an input menu, which is a tree structure of input data, where data items (parameters) are organized hierarchically in submenus. Each data item is associated with a name, default value, unit, help text, widget type, validation information, etc. Different types of sophisticated user interfaces can then be automatically generated: a graphical web interface (via Flask or Django), a command-line interface, and a file-based interface. The tutorial describes specific examples on how to to program Parampool to generate user interfaces and how to operate them. With very little efforts, you can take a scientific application and equip it with a fancy GUI.

NOTE: This report is in a **very preliminary state**, but should be sufficient for exploring Parampool for creating web GUIs. Please send email to the first author for questions, reporting typos and errors, request of more information, etc.

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2DO.

- \bullet More links to additional material: (Read these when returning to this work)
 - Quick Flask++ tutorial
 - Quick overview of Bootstrap 3, another Bootstrap 3 tutorial
 - Flask and Boostrap intro (sample app has sign in functionality and bootstrap layout explained here)
 - Flask, Heroku and Bootstrap (this is a good recipe we can turn into building a science app)
 - Facebook login in Flask
 - Flask-Bootstrap and its doc, read in particular basic usage and see the (only?) example
 - Bootstrap video intro

- A complete modern Python project with virtualenv, testing, setup.py, etc.
- Skulpt: Interactive Python in the browser
- Python for computer games

1 Simulation program

We shall work with a sample application that takes a few variables as input and produces numbers and/or graphs as result. Specifically, our application, later referred to as a *simulation program* or simply a *simulator*, concerns the simulation of a ball thrown through air. Given the initial velocity of the ball, and some other data like mass and radius, we can compute the trajectory of the ball until it hits the ground. The details of the calculations are not of interest here as our focus is on software for assigning input data and for displaying the results. However, the interested reader can consult the box below for the inner workings of the simulation program.

Mathematical model.

The motion of the mass center r of a body through a fluid is given by

$$m\frac{d^2\mathbf{r}}{dt^2} = -m\mathbf{g} - \frac{1}{2}C_D\varrho Av^2\mathbf{i}_t + \frac{1}{2}C_L\varrho Av^2\mathbf{i}_n + \frac{1}{2}C_S\varrho Av^2(\mathbf{i}_t \times \mathbf{i}_n), \quad (1)$$

where m is the mass of the body, \boldsymbol{g} is the acceleration of gravity vector, C_D is a drag coefficient, ϱ is the density of air, A is the cross-section area of the body perpendicular to the motion, $v = |\boldsymbol{v} - \boldsymbol{w}|$ is the relative velocity between the body, $\boldsymbol{v} = d\boldsymbol{r}/dt$, and a given wind velocity \boldsymbol{w} , C_L is a lift coefficient, C_S is a coefficient for the sidewind or lateral aerodynamic force, \boldsymbol{i}_t is a unit tangent vector of the body's path, while \boldsymbol{i}_n is a unit vector normal to the path tilting upwards. The drag C_D coefficient for a sphere is taken as 0.45. The lift coefficient C_L depends on the spinrate ω (rad s⁻¹) of the body, and a simple linear relation often suffices: $C_L = 0.2\omega/500$. A negative ω gives a negative lift.

We can simplify the model for a two-dimensional motion in an xy plane with unit vectors \boldsymbol{i} and \boldsymbol{j} in the x and y directions, respectively. Then we skip the sidewind force $(C_S = 0)$. We also let gravity point downwards, $\boldsymbol{g} = -g\boldsymbol{j}$, and let the wind velocity be horizontal: $\boldsymbol{w} = -w\boldsymbol{i}$. Furthermore, we have that

$$i_t = \frac{\mathbf{v}}{|\mathbf{v}|} \equiv a\mathbf{i} + b\mathbf{j}, \quad \mathbf{v} = \frac{d\mathbf{r}}{dt},$$
 (2)

$$\mathbf{i}_n = -b\mathbf{i} + a\mathbf{j} \text{ if } a > 0 \text{ else } b\mathbf{i} - a\mathbf{j}$$
(3)

The initial conditions associated with (1) express that the body starts at the origin with an initial velocity v_0 making an angle θ with the horizontal. In the two-dimensional case the conditions become

$$r(0) = 0\mathbf{i} + 0\mathbf{j}, \quad \frac{d\mathbf{r}}{dt}(0) = \mathbf{v}(0) = v_0 \cos \theta \mathbf{i} + v_0 \sin \theta \mathbf{j}.$$

2 User interfaces for Python functions

Parampool can automatically generate user interfaces for communicating with a given function. The usage of this functionality will be explained in problems of increasing complexity, using the trajectory of a ball as described above as application.

2.1 Real numbers as input and output

Suppose you have some function

```
def compute_drag_free_landing(initial_velocity, initial_angle):
    ...
    return landing point
```

This function returns the landing point on the ground (landing_point) of a ball that is initially thrown with a given velocity in magnitude (initial_velocity), making an angle (initial_angle) with the ground. There are two real input variables and one real output variable. The function must be available in some module, here the module is simply called compute.py (and it also contains a lot of other functions for other examples).

In the following we shall refer to functions like compute_drag_free_landing, for which we want to generate a web interface, as a *compute function*.

Flask interface. Flask is a tool that can be used to write a graphical user interface (GUI) to be operated in a web browser. Here we shall use Flask to create a GUI for our compute function, as displayed in Figure 1. To this end, simply create a Python file generate.py with the following lines:

```
from parampool.generator.flask import generate
from compute import compute_drag_free_landing
generate(compute_drag_free_landing, default_field='FloatField')
```

The generate function grabs the arguments in our compute function and creates the necessary Flask files.

Input:

Results:



Figure 1: A simple web interface.

Tip.

We recommend to make a new directory for every web application. Since you need access to the compute module you must copy compute.py to the directory or modify PYTHONPATH to contain the path to the directory where compute.py resides.

Since the generate tool has no idea about the type of variable of the two positional arguments in the compute function, it has to assume some type. By default this will be text, but we can change that behavior to be floats by the setting the default_field argument to FloatField. This means that the generated interface will (only) accept float values for the input variables, which is sufficient in our case.

A graphical Flask-based web interface is generated by running

Terminal> python generate.py

Warning.

A message is written in the terminal window, saying that with positional arguments in the compute function, one must normally invoke the generated controller.py file and do some explicit conversion of text read from the web interface to the actual variable type accepted by the compute function. This potential manual work can be avoided by using keyword arguments only, so the generator functionalty can see the variable type.

You can now view the generated web interface by running

Terminal> python controller.py

and open your web browser at the location http://127.0.0.1:5000/. Fill in values for the two input variables and press *Compute*. The page in the Chrome browser will now look like Figure 1. Other browsers (Firefox, for instance) may have a slightly different design of the input fields. All figures in this tutorial are made with the Chrome browser.

Generated files:

Readers with knowledge of Flask will notice that some files with Flask code have been generated:

- model.py with a definition of the forms in the web interface
- controller.py which glues the interface with the compute function
- templates/view.html which defines the design of the web interface

You are of course free to tailor these files to your needs if you know about Flask programming. An introduction to Flask for scientific applications is provided in [?]. A one-line Bash script, clean.sh, is also generated: it will remove all files that were generated by running generate.py.

Django interface. Django is a very widespread and popular programming environment for creating web applications. We can easily create our web application in Django too. Just replace flask by django in generate.py:

```
from parampool.generator.django import generate
from compute import compute_drag_free_landing
generate(compute_drag_free_landing, default_field='FloatField')
```

The Django files are now in the directory tree drag_free_landing (same name as our compute function, except that any leading compute_ word is removed). Run the application by

```
Terminal> python drag_free_landing/manage.py runserver
```

and open your browser at the location http://127.0.0.1:8000/. The interface looks the same and has the same behavior as in the Flask example above.

Generated files:

Quite some files are needed for a Django application. These are found in the drag_free_landing directory tree. The most important ones are

- models.py with a definition of the forms in the web interface
- views.py which glues the interface with the compute function

• templates/index.html which defines the design of the web interface

With some knowledge of basic Django programming you can edit these files to adjust the functionality. Reference [?] provides a basic introduction to Django for creating scientific applications.

2.2 A plot as output

The result of the previous computation was just a number. Let us instead make a plot of the trajectory of a ball without any air resistance. The function

```
def compute_drag_free_motion_plot(
   initial_velocity=5.0,
   initial_angle=45.0):
   ...
   return html text
```

is now our compute function, in compute.py, which takes the same two input arguments as before, but returns some HTML text that will display a plot in the browser window. This HTML text is basically the inclusion of the image file containing the plot,

```
<img src="X">
```

where X is the name of the file. However, if you do repeated computations, the name of the image file must change for the browser to update the plot. Inside the compute function we must therefore generate a unique name of each image file. For this purpose, we can use the number of seconds since the Epoch (January 1, 1970) as part of the filename, obtained by calling time.time(). In addition, the image file must reside in a subdirectory static. The appropriate code is displayed below.

```
import matplotlib.pyplot as plt
...

def compute_drag_free_motion_plot(
    initial_velocity=5.0,
    initial_angle=45.0):
    ...

plt.plot(x, y)
    import time # use time to make unique filenames
    filename = 'tmp_%s.png' % time.time()
    if not os.path.isdir('static'):
        os.mkdir('static')
    filename = os.path.join('static', filename)
    plt.savefig(filename)
    html_text = '<img src="%s" width="400">' % filename
    return html_text
```

The string version of the object returned from the compute function is inserted as *Results* in the HTML file, to the right of the input. By returning the appropriate HTML text the compute function can tailor the result part of the page to our needs.

Figure 2: A web interface with graphics.

Flask application. The generate.py file for this example is similar to what is shown above. Only the name of the compute function has changed:

```
from parampool.generator.flask import generate
from compute import compute_drag_free_motion_plot
generate(compute_drag_free_motion_plot)
```

Tip.

This time we do not need to specify default_field because we have used keyword arguments with default values in the compute function. The generate function can then from the default values see the type of our arguments. Remember to use float default values (like 5.0) and not simply integers (like 5) if the variable is supposed to be a float.

We run python generator.py to generate the Flask files and then python controller.py to start the web GUI. Now the default values appear in the input fields. These can be altered, or you can just click *Compute*. The computations result in a plot as showed in Figure 2.

Django application. The corresponding Django application is generated by the same generator.py code as above, except that tword flask is replaced by django. The Django files are now placed in the drag_free_motion_plot subdirectory, and the web GUI is started by running

Terminal> python drag_free_motion_plot/manage.py runserver

The functionality of the GUI is identical to that of the Flask version.

Comparing graphs in the same plot. With a little trick we can compare several trajectories in the same plot: inserting plt.figure(X) makes all plt.plot calls draw curves in the same figure (with figure number X). We introduce a boolean parameter new_plot reflecting whether we want a new fresh plot or not,

The new_plot parameter will turn up as a boolean variable in the web interface, and when checked, we create a new figure. Otherwise, we draw curves in the existing figure number fig_no which was initialized last time new_plot was true (with a global variable we ensure that the value of fig_no survives between the calls to the compute function). Figure 3 displays an attempt to not check new_plot and compare the curves corresponding to three different parameters (the files are in the 'flask3 directory.

Caveat.

If new_plot is unchecked before the first computation is carried out, fig_no is not defined when we do plt.figure(fig_no) and we get a NameError exception. A fool-proof solution is

```
if new_plot:
    fig_no = plt.figure().number
else:
    try:
        plt.figure(fig_no)
    except NameError:
        fig_no = plt.figure().number
```

Avoiding plot files.

Figure 3: Plot with multiple curves.

The compute function generates plot files with unique names, but we can avoid making files at all and just insert the PNG code of the plot, using base64 encoding, as a long string directly in the HTML image tag. The statements below sketches the idea:

There is a convenient function parampool.utils.save_png_to_str performing the statements above and returning the html_text string:

```
from parampool.utils import save_png_to_str
# make plot in plt (matplotlib.pyplot) object
html_text = save_png_to_str(plt, plotwidth=400)
```

With this construction one can very easily avoid plot files and embed the plot directly in the HTML code.

Matplotlib without X server.

Matplotlib is by default configured to work with a graphical user interface which may require an X11 connection. When running applications on a web server there is a possibility that X11 is not enabled, and the user will get an error message. Matplotlib thus needs to be configured for use in such environments. The configuration depends on what kinds of images the user wants to generate, but in most cases it is sufficient to use the Agg backend. The Agg backend is created to make PNG files, but it also recognizes other formats like PDF, PS, EPS and SVG. The backend needs to be set before importing pyplot or pylab:

```
import matplotlib as mpl
mpl.use('Agg')
import matplotlib.pyplot as plot
```

2.3 More input parameters and results

It is time to address a more complicated application: we want to compute the trajectory of a ball subject to air drag and lift and compare that trajectory to the one where drag and lift are omitted. We also want to visualize the relative importance between the three forces: gravity, drag, and lift. The lift is caused by spinning the ball.

The function that performs the computations has the following signature:

```
def compute_motion_and_forces0(
   initial_velocity=5.0,
   initial_angle=45.0,
   spinrate=50.0,
   w=0.0,
   m=0.1,
   R=0.11,
   method='RK4',
   dt=None,
   plot_simplified_motion=True,
   new_plot=True
   ):
```

and returns a formatted string html_text with two plots organized as a table. The technique described in the *Avoiding plot files* box at the end of Section pp:plot:output is implemented to embed PNG images directly in the HTML code. Under the plots there is a table of input values and the landing point. Curves can be accumulated in the plots (new_plot=True), with the corresponding data added to the table. A rough sketch of the HTML code returned from the compute function goes as follows:

```
<img src="data:image/png;base64,iVBORwOKGgoAAAA..." width="400">
```

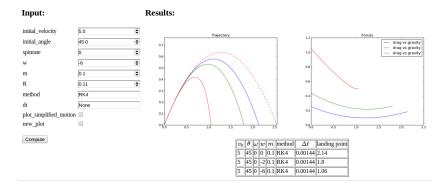


Figure 4: Web interface with two graphs.

```
<img src="data:image/png;base64,iVBORwOKGgoAAAA..." width="400">
<center>
<t.r>
 \( v_0 \) 
 \( \theta \) 
 \( \omega \) 
 \( w \)
           \( m \)
           \( R \)
           method
           \( \Delta t \) 
 landing point 
 5  45  ...
</center>
```

Note that we use MathJax syntax for having LATEX mathematics in the table heading. All details about the computations and the construction of the returned HTML string can be found in the compute.py file.

Any doc string of the compute function is copied and typeset verbatim at the top of the web interface. However, if the text # (DocOnce format) appears somewhere in the doc string, the text is taken as DocOnce source code and translated to HTML, which enables typesetting of LATEX mathematics and computer code snippets (with nice pygments formatting).

The documentation of the web interface can therefore be included as a doc string in the compute function. Here is descriptive doc string using DocOnce syntax for LATEX mathematics (equations inside !bt and !et commands) and

monospace font for Python variables (names in backticks). The corresponding view in a browser is shown in Figure 5.

..

This application computes the motion of a ball with radius R and mass m under the influence of gravity, air drag and lift because of a given spinrate ∞ . The motion starts with a prescribed initial velocity v_0 making an angle initial_angle theta\$ with the ground. A wind velocity w, positive in positive x direction, can also be given.

The ordinary differential equation problem governing the motion reads

```
!bt \begin{align*} m\frac{d^2\bm{r}}{dt^2} &= -mg\bm{j} - \frac{1}{2}C_D\varrho A v^2\bm{i}_t + \frac{1}{2}C_L\varrho A v^2\bm{i}_n\\bm{r}(0) &= 0\bm{i} + 0\bm{j}\\frac{d\bm{r}}{dt}(0) &= v_0\cos\theta\bm{i} + v_0\sin\theta\bm{j}, \end{align*} !et where $\bm{i}$ and $\bm{j}$ are unit vectors in the $x$ and $y$ directions, respectively, $g$ is the acceleration of gravity, $A$ is the cross section area normal to the motion, $\bm{i}_t$ is a unit tangent vector to the trajectory, $\bm{i}_n$ is a normal vector (pointing upwards) to the trajectory, $C_D$ and $C_L$ are lift coefficients, and $\varrho$ is the air density. For a ball, $C_D$ is taken as 0.45, while $C_L$ depends on the spinrate through $C_L=0.2\omega/500$.
```

Many numerical methods can be used to solve the problem. Some legal names are 'ForwardEuler', 'RK2', 'RK4', and 'Fehlberg' (adaptive Runge-Kutta 4/5 order). If the timestep 'dt' is None, approximately 500 steps are used, but 'dt' can also be given a desired 'float' value.

The boolean variable 'plot_simplified_motion' adds the curve of the motion without drag and lift (the standard parabolic trajectory). This curve helps illustrate the effect of drag and lift. When 'new_plot' is 'False' (unchecked), the new computed curves are added to the previous ones since last time 'new_plot' was true.

```
# (DocOnce format)
"""
```

The generate.py code for creating the web GUI goes as in the other examples,

```
from parampool.generator.flask import generate
from compute import compute_motion_and_forces
generate(compute_motion_and_forces, MathJax=True)
```

and we start the application as usual by python controller.py. The resulting web interface appears in Figure 4. The table shows the sequence of data we have given; starting with the default values, then turning off the

This application computes the motion of a ball with radius R and mass m under the influence of gravity, air drag and lift because of a given spinrate ω . The motion starts with a prescribed initial velocity v_0 making an angle initial_angle θ with the ground. A wind velocity w_0 positive in positive z direction, can also be given.

The ordinary differential equation problem governing the motion reads

$$\begin{split} & m \, \frac{d^2 \boldsymbol{r}}{dt^2} = - m \boldsymbol{g} \boldsymbol{j} - \frac{1}{2} \, C_D \varrho A \boldsymbol{v}^2 \boldsymbol{i}_t + \frac{1}{2} \, C_L \varrho A \boldsymbol{v}^2 \boldsymbol{i}_n \\ & \boldsymbol{r}(0) = 0 \boldsymbol{i} + 0 \boldsymbol{j} \\ & \frac{d \boldsymbol{r}}{dt} \, (0) = v_0 \cos \theta \boldsymbol{i} + v_0 \sin \theta \boldsymbol{j}, \end{split}$$

where i and j are unit vectors in the x and y directions, respectively, g is the acceleration of gravity, A is the cross section area normal to the motion, i_t is a unit tangent vector to the trajectory, i_t is a normal vector (pointing upwards) to the trajectory, C_D and C_L are lift coefficients, and ϱ is the air density. For a ball, C_D is taken as 0.45, while C_L depends on the spinrate through $C_L = 0.2\omega/500$.

Many numerical methods can be used to solve the problem. Some legal names are ForwardEuler, RK2, RK4, and Fehlberg (adaptive Runge-Kutta 4/5 order). If the timestep dt is None, approximately 500 steps are used, but dt can also be given a desired float value.

The boolean variable plot_simplified_motion adds the curve of the motion without drag and lift (the standard parabolic trajectory). This curve helps illustrate the effect of drag and lift. When new_plot is False (unchecked), the new computed curves are added to the previous ones since last time new_plot was true.

Figure 5: Web interface with documentation.

plot_simplified_motion curve and new_plot, then running two cases with different values for the wind parameter w. The plot clearly show the influence of drag and wind against the motion.

MathJax.

The compute_motion_and_forces function returns mathematical symbols in the heading line of the table with data. MathJax must be enabled in the HTML code for these symbols to be rendered correctly. This is specified by the MathJax=True argument to generate. (However, in this particular example MathJax is automatically turned on since we use DocOnce syntax and mathematics in the doc string.)

Django interface. As before, the Django interface is generated by importing the function generate from parampool.generator.django. A subdirectory motion_and_forces contains the files, and the Django application is started as shown in previous examples and has the same functionality as the Flask application.

2.4 Other types of function arguments

The generate function will recognize the following different types of keyword arguments in the compute function: float, int, bool, str, list, tuple, numpy.ndarray, name of a file, as well as user-defined class types (a la MySpecialClass). Here is a minimalistic example on computing the mean and standard deviation of data either in an array or in a file (we use the file if the operator of the web interface assigns a file to filename):

```
def compute_average(data_array=np.array([1]), filename=None):
    if filename is not None:
        data = np.loadtxt(os.path.join('uploads', filename))
        what = 'file %s' % filename
    else:
```

Input: data_array [1] filename Choose File No file chosen Compute Results: Data from file mydata.dat: mean 0.236 st.dev. 0.604

Figure 6: Web interface for uploading a file.

The output is simple, basically two numbers in a table and an intro line.

We write a generate.py file as shown before, but with compute_average as the name of the compute function. For any argument containing the string filename it is assumed that the argument represents the name of a file. The web interface will then feature a button for uploading the file.

When the application runs, we have two data fields: one for setting an array with list syntax and one for uploading a file. Clicking on the latter and uploading an file mydata.dat containing just columns of numbers, results in the web page displayed in Figure 6. In this case, when a filename was assigned, we use the data in the file. Alternatively, we can instead fill in the data array and click Compute, which then will compute the basic statistics of the assigned data array.

3 Working with a menu of input parameters

Parampool's main focus is on scientific applications with lots of input data of different type, organized in a hierarchical tree fashion. The various input parameters are defined in terms of a *menu*. The menu can be defined as a nested list or through function application programming interface (known as an API, and here consisting of calls functionality in the parampool.menu package).

To exemplify the use of menus, we apply the $compute_motion_and_forces$ function (from Section 2.3):

```
def compute_motion_and_forces0(
   initial_velocity=5.0,
```

```
initial_angle=45.0,
spinrate=50.0,
w=0.0,
m=0.1,
R=0.11,
method='RK4',
dt=None,
plot_simplified_motion=True,
new_plot=True
).
```

Let us organize 10 input parameters into four submenus. At the top level we need a submenu, usually called "Main menu" or named after the application. Each submenu is here specified with a logical name of each parameter and the corresponding variable names in the compute function:

• Main menu

```
- Initial motion data
```

```
* Initial velocity: initial_velocity
* Initial angle: initial_angle
```

* Spinrate: spinrate

- Body and environment data

```
* Wind velocity: w
```

* Mass: m * Radius: R

- Numerical parameters

* Method: method * Time step: dt

- Plot parameters

* Plot simplified motion: plot_simplified_motion

* New plot: new_plot

With a menu we can give the parameters more readable logical names (not restricted to a valid variable name in Python), but we can also specify a lot other properties too, as will be explained.

A menu is a hierarchical tree structure with submenus and data items, where each data item describes an input parameter in the problem. The task now is to make a Python specification of the of submenus and data items in the menu tree.

3.1 Specify a menu as a list

The menu tree can be specified as a list of lists, strings, and dictionaries. Each list represents a submenu, each string the name of the submenu, and each dict is a data item. The menu must be return from some function, hereafter called the *menu function*. In our case, the menu function goes as follows:

```
def menu_definition_list():
     """Create and return menu defined through a nested list."""
    menii = \Gamma
         'Main', [
             'Initial motion data', [
                  dict(name='Initial velocity', default=5.0),
                  dict(name='Initial angle', default=45,
                       widget='range', minmax=[0,90], range_step=1),
                  dict(name=r'Spinrate', default=50, widget='float',
                       unit='1/s'),
             'Body and environment data', [
                  dict(name='Wind velocity', default=0.0,
                       help='Wind velocity in positive x direction.',
                       minmax=[-50, 50], number_step=0.5,
                       widget='float', str2type=float),
                  dict(name='Mass', default=0.1, unit='kg',
                       validate=lambda data_item, value: value > 0,
                       help='Mass of body.'),
                  dict(name='Radius', default=0.11, unit='m',
                       help='Radius of spherical body.'),
             'Numerical parameters', [
dict(name='Method', default='RK4',
                       widget='select',
options=['RK4', 'RK2', 'ForwardEuler'],
                       help='Numerical solution method.'),
                  dict(name='Time step', default=None,
     widget='textline', unit='s'),
                 ],
             'Plot parameters', [
                  dict(name='Plot simplified motion', default=True,
                       help='Plot motion without drag+lift forces.'),
                  dict(name='New plot', default=True,
    help='Erase all old curves.'),
                  ],
             ],
        ]
    from parampool.menu.UI import listtree2Menu
    menu = listtree2Menu(menu)
    return menu
```

Actually, the menu function must return a parampool.menu.Menu object, so after the definition of the menu tree as a list we must make the shown conversion from a list to Menu object via the listtree2Menu function.

3.2 Attributes in data items

Each data item has a name and preferably a default value, as in the case of "Initial velocity". More attributes can be added:

- 'widget' specifies the type of widget used in a graphical user interface. Legal values are integer, float, range (requires the minmax attribute), integer_range (requires the minmax attribute), textline, textarea (for larger multi-line texts), checkbox (for boolen variables), select (list of options), email, password, file (for a filename of a file to be uploaded, url, hidden (for an invisible field), and tel (for a phone number). If not given, widget is based on the value of str2type or the type of the default value.
- minmax is a 2-list or 2-tuple with lower and upper bound in the interval of legal values of a number.
- The range_steps attribute, valid when widget is range, specifies the steps in the slider used to select the number. Here we can select the "Initial angle" in unit steps between 0 and 90 degrees.
- unit specifies a unit, e.g., 1/s or kg/m**3, or 1/s.
- help adds a help string to explain more about the parameter and how it can be set.
- number_step specifies the precision of float or integer widgets if minmax is also specified (default 0.001), otherwise the precision is arbitrary.
- str2type is a conversion function from a string (text given in a user interface) to the right type for the parameter. A value is automatically assigned if widget is given, otherwise one applies the default value to find the right str2type function. This means that it is strictly not necessary to assign for the "Wind velocity" data item. With more complicated objects one can assign a user-given conversion function to str2type (shown later).
- option is a list of options for a select widget, here the type of numerical solution methods that can be chosen.
- validate holds a function that takes the value of the data item as argument and returns True or False depending on whether the value can be accepted or not.
- symbol contains a mathematical LATEX symbol that will be used in Flask or Django interfaces instead of the name of data item.
- widget_size specifies the size (width) of fields in graphical user interfaces.
- textline must be used for default values that are None, because another value or the text "None" can be written in the field. In this case, str2type is automatically set to eval and any valid Python expression is then essentially allowable, but wrong objects will give errors in the compute function.

3.3 The compute function

When working with menus, the compute function is allowed to take *only one* argument called menu. This object is used to extract input data. Basically, the value of any data item my parameter in the menu is extracted by

```
variable = menu.get_value('my parameter')
```

In case multiple data items have the same name, enough of the submenu path must be given, e.g.,

```
variable = menu.get_value('My Submenu1/my parameter')
```

Our specific computing function is a wrapper for compute_motion_and_forces:

```
def compute_motion_and_forces_with_menu(menu):
    initial_velocity = menu.get_value('Initial velocity')
    initial_angle = menu.get_value('Initial angle')
    spinrate = menu.get_value('Spinrate')
    w = menu.get_value('Wind velocity')
    m = menu.get_value('Mass')
    R = menu.get_value('Mass')
    method = menu.get_value('Method')
    dt = menu.get_value('Time step')
    plot_simplified_motion = menu.get_value('Plot simplified motion')
    new_plot = menu.get_value('New plot')
    return compute_motion_and_forces(
        initial_velocity, initial_angle, spinrate, w,
        m, R, method, dt, plot_simplified_motion,
        new_plot)
```

The assumption is that the menu object provides enough input data for the compute function. If this assumption does not hold, one can simply make a class, store extra data as attributes in the class, and let the compute function be a method in the class.

3.4 Generating a user interface

With a menu function and a compute function at hand, it remains to make a new directory, copy the module(s) containing the menu function and compute function to this directory, and write a generate.py file with the content

The generate function will now use the information in the menu (and not the arguments in the compute function!) to generate a flexible user interface. Note that an Internet connection is required. After running

```
Terminal> python generate.py
```



Figure 7: Web interface in closed form.

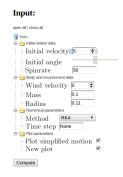


Figure 8: Web interface in fully expanded form.

several Flask files and directories are generated (model.py, controller.py, templates, static, and a simple clean-up script clean.sh). The user interface is started by

```
Terminal> python controller.py
```

Open the URL http://127.0.0.1:5000 in a web broswer to see an interface as the one in Figure 7.

3.5 Operating the user interface

The menu tree is mapped onto a visual structure often used for directory trees. Clicking on *open all* at the top of the user interface expands all submenus so that all parameters (data items) become visible. Figure 8 displays the result in the Opera browser. Note that in this type of user interface, the name of each data item is typeset in IATEX and inserted as a picture.

The following technical points must be mentioned.

- A plain float or integer value gives a textline widget, while if a minmax range is specified, a float or integer widget (HTML5 number field) is chosen. Choosing float or integer explicitly as widget may lead to different width of the widget in different browsers.
- 2. Data items whose widgets are specified as float or integer, or where this is implied because str2type is float or int, or the default value is

a float or int and the minmax attribute is assign, are shown using the HTML5 input field called number. This is recogned by the small (and not so useful) arrows that can be used to adjust the number, but usually typing in the number manually is faster and more precise. An extra attribute, number_step controls the stepping when clicking on the arrows and also the allowed precision of a typed number (same as number_step, which by default is 0.001).

- 3. When the widget is range, an HTML5 range field is used, which is usually rendered as a slider in browsers. The slider gets by default 100 steps (can be changed or specified individually for any data item).
- 4. With the select widget we get a pull-down menu with the different options.
- Any data item whose default value is True or False maps directly to a checkbox for boolean parameters.
- 6. Any data item with unit specified maps to an ordinary text field, since input consists of a number with an optional text for the unit. That is, if we choose to set unit='m/s' for the "Initial velocity" data item, the input field will not the an HTML5 number field, but a standard HTML text field.
- 7. The names of the data items are typeset in LATEX and shown as PNG images. This means that data item names may contain mathematical expressions: Spinrate \$\omega\$ for instance.

Warning.

The HTML5 number field is rendered differently in different browsers. This can lead to strange layout of the input fields. In such cases it is recommended to avoid the HTML5 number field. This is easiest accomplished by explicitly specifying widget to be textline. This is also the default widget type if you equip the number with a unit or do not specify any widget, just a float or integer default value.

We can try out the interface:

- 1. Set "Initial velocity" to 8.
- 2. Move the slider for "Initial angle" to 55.
- 3. Add a positive "Wind velocity" of -3.
- 4. Specify "Mass" as the text 0.1*1000 g (i.e., we use g rather than the default kg as unit, but the value is still 0.1 kg).
- 5. Choose RK2 for "Method".



Figure 9: Web interface with input parameters filled out.

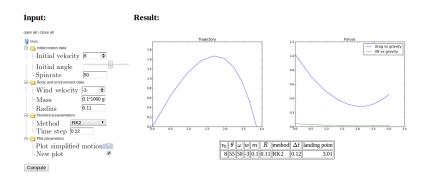


Figure 10: Web interface with input and results.

- 6. Set "Time step" to 0.12.
- 7. Uncheck the "Plot simplified motion" boolean value.
- 8. Hold the mouse pointer over the "Wind velocity" field to see the help string. Then point the mouse to "Mass" input field and the specified unit pops up. A combination of help and unit information is showed if both are given in the data item definition.

You should see something like Figure 9.

Now, press the *Compute* button. Figure 10 shows the resulting response. You can now play around and click the checkbox for *Plot simplified motion* and the recompute to see the effects of wind against the motion, drag, and lift (which are substantial in this example).

3.6 Detection of wrong input

Text in a number field. Write abc in the "Initial velocity" field and press the *Compute* button. The error message "Please enter a number" pops up.

Failure of user-provided validate function. Give a negative value for "Mass". The "Mass" data item has a validation function provided by us. A False value returned from this function gives rise to a DataItemValueError shown in the browser. It reads here Mass = -0.1: validate function <lambda> claims invalid value.

Failure of converting string to right type. Write abc for "Radius". This is a text field so any text is in principle valid, but parampool raises a TypeError with the message could not apply str2type=<type 'float'> to value abc <type 'str'>.

Failure in the compute function. Give a list [0.1, 0.2] for "Time step". Since the default is None, which causes str2type=eval, any Python expression is accepted in the interface, but the compute function raises a TypeError because float(dt) fails when dt is a list. A remedy is to write a tailored str2type function:

Setting str2type=convert_time_step for the "Time step" data item gives an informative error message if the answer is not as expected: None or a floating-point number.

3.7 Specifying a menu using an API

Instead of listing all the entries in the menu tree as strings, lists, and dicts in a nested data structure, you can use the Application Programming Interface (API) of the parampool.menu package. The menu defined above is alternatively programmed like this using the API:

```
# Move to (and create) another submenu, as in a file tree
menu.submenu('../Body and environment data')
# Add data items for the current submenu
menu.add_data_item(
    name='Wind velocity', default=0.0,
    help='Wind velocity in positive x direction.',
    minmax=[-50, 50], number_step=0.5,
widget='float', str2type=float)
menu.add_data_item(
    name='Mass', default=0.1, unit='kg',
    validate=lambda data_item, value: value > 0,
    help='Mass of body.')
menu.add_data_item(
    name='Radius', default=0.11, unit='m',
    help='Radius of spherical body.')
menu.submenu('../Numerical parameters')
menu.add_data_item(
    name='Method', default='RK4',
    widget='select',
options=['RK4', 'RK2', 'ForwardEuler'],
help='Numerical solution method.')
menu.add_data_item(
    name='Time step', default=None,
widget='textline', unit='s', str2type=convert_time_step)
menu.submenu('../Plot parameters')
menu.add_data_item(
    name='Plot simplified motion', default=True,
    help='Plot motion without drag+lift forces.')
menu.add_data_item(
    name='New plot', default=True,
    help='Erase all old curves.')
menu.update()
return menu
```

The API is in many ways easier to use than the nested data structure with lists, strings, and dicts. The API resembles moving around in a file tree. The rules are simple:

- menu. submenu(path) moves us to a submenu path, and creates it first if it does not exist. This is similar to cd path in a file tree, or mkdir path; cd path, if path does not exist.
- The name of a submenu, path, follows the rule of file and directory names in a file tree: a slash is used as delimiter between submenus and data items. For example:
 - -/Main menu/Initial motion data/Initial velocity is the full path to the "Initial velocity" data item.
 - Standing in the "Initial motion data" submenu, .. is the parent submenu ("Main menu"), while ../Numerical parameters is the correct path to the "Numerical parameters" submenu. That is, we can use relative and absolute paths as in a file tree.

• A data item is appended to the current submenu by calling menu.add_data_item.

The look and functionality of this GUI (found in the flask_menu2 directory) are the same as in the previous one (found in the flask_menu1 directory).

3.8 Specifying a menu using an alternative API

There is an another syntax for defining submenus as well:

```
def menu_definition_api_with_separate_submenus():
    Create and return a menu by calling up other functions
    for defining the submenus. Also demonstrate customization
    of menu properties and inserting default values from file
    or the command line.
    from parampool.menu.Menu import Menu
    menu = Menu()
    menu.submenu('Main menu')
    menu = motion_menu(menu)
    menu.change_submenu('...')
    menu = body_and_envir_menu(menu)
    menu.change_submenu('...')
    menu = numerics_menu(menu)
    menu.change_submenu('..')
    menu = plot_menu(menu)
    menu.update() # finalize menu construction
    from parampool.menu.UI import (
        set_data_item_attribute,
        set_defaults_from_file,
        set_defaults_from_command_line,
set_defaults_in_model_file,
        write_menufile,
    # Change default values in the web GUI
    import parampool.menu.DataItem
    parampool.menu.DataItem.DataItem.defaults['minmax'] = [0, 100]
    parampool.menu.DataItem.DataItem.defaults['range_steps'] = 500
    # Can also change 'number_step' for the step in float fields
    # and 'widget_size' for the width of widgets
    # Let all widget sizes be 6, except for Time step
    menu = set_data_item_attribute(menu, 'widget_size', 6)
    menu.get('Time step').data['widget_size'] = 4
    menu = set_defaults_from_file(menu, command_line_option='--menufile')
    menu = set_defaults_from_command_line(menu)
    flask_modelfile = 'model.py'
    django_modelfile = os.path.join('motion_and_forces_with_menu', 'app',
                                     'models.py')
    if os.path.isfile(flask modelfile):
        set_defaults_in_model_file(flask_modelfile, menu)
    elif os.path.isfile(django_modelfile):
        set_defaults_in_model_file(django_modelfile, menu)
    menufile = open('menu.dat', 'w')
    menufile.write(write_menufile(menu))
    menufile.close()
```

```
return menu
def motion_menu(menu, name='Initial motion data'):
    menu.submenu(name)
    menu.add_data_item(
        name='Initial velocity', default=5.0, symbol='v_0',
        unit='m/s', help='Initial velocity',
        str2type=float, widget='float',
        validate=lambda data_item, value: value > 0)
    menu.add_data_item(
        name='Initial angle', default=45, symbol=r'\theta',
        widget='range', minmax=[0,90], str2type=float,
        help='Initial angle',
        validate=lambda data_item, value: 0 < value <= 90)</pre>
    menu.add_data_item(
        name='Spinrate', default=50, symbol=r'\omega',
widget='float', str2type=float, unit='1/s',
help='Spinrate')
    return menu
def body_and_envir_menu(menu, name='Body and environment data'):
    menu.submenu(name)
    menu.add_data_item(
        name='Wind velocity', default=0.0, symbol='w',
        help='Wind velocity in positive x direction.', unit='m/s',
        minmax=[-50, 50], number_step=0.5,
    widget='float', str2type=float)
menu.add_data_item(
        name='Mass', default=0.1, symbol='m',
        help='Mass of body.', unit='kg',
        widget='float', str2type=float,
        validate=lambda data_item, value: value > 0)
    menu.add_data_item(
        name='Radius', default=0.11, symbol='R',
        help='Radius of spherical body.', unit='m',
        widget='float', str2type=float,
        validate=lambda data_item, value: value > 0)
    return menu
def numerics_menu(menu, name='Numerical parameters'):
    menu.submenu(name)
    menu.add_data_item(
        name='Method', default='RK4',
widget='select',
options=['RK4', 'RK2', 'ForwardEuler'],
        help='Numerical solution method.')
    menu.add_data_item(
        name='Time step', default=None, symbol=r'\Delta t',
        widget='textline', unit='s', str2type=eval,
        help='None: ca 500 steps, otherwise specify float.')
    return menu
def plot menu(menu, name='Plot parameters'):
    menu.submenu(name)
    menu.add_data_item(
        name='Plot simplified motion', default=True,
        help='Plot motion without drag and lift forces.')
    menu.add_data_item(
        name='New plot', default=True,
```

```
help='Erase all old curves.')
return menu
```

This code contains three important additional features:

- 1. documentation of the application is in an external file doc.html
- 2. the name of a parameter can be a mathematical symbol
- 3. parameters can have multiple values for investigating many parameter sets at once

File with documentation of the application. We have in Section 2.3 seen that the doc string of the compute function may contain a mathematical description of the problem with rich typesetting (using DocOnce syntax). It is also possible to make such a description in a separate file. Any HTML file will work, and the filename is specified by the doc argument to generate.

LATEX symbol as parameter name. One can add a mathematical LATEX symbol for the parameter names (the symbol keyword argument). This symbol can either be displayed as the parameter's complete name, or the symbol can be added to the standard name of the parameter. The choice is set by the latex_name keyword argument in the generate call in generate.py:

The values of latex_name can be 'symbol' (symbol only) or 'text, symbol' (ordinary name followed by a comma and the symbol).

Multiple input values for parameters. We can specify multiple values for parameters whose input fields are pure text fields. For example, for the wind velocity (w) parameter we can assign two values separated by the & character: 0 & -8. Calling menu.get_values('Wind velocity') will then return a list [0, -8] rather than one number. We can hence easily make a loop over the multiple values for each parameter where we use pure text as input. Our compute function looks in this case like this:

```
def compute_motion_and_forces_with_menu_loop(menu):
    html = ''
    initial_angle = menu.get_value('Initial angle')
    method = menu.get_value('Method')
    new_plot = menu.get_value('New plot')  # should be True here
    plot_simplified_motion = menu.get_value('Plot simplified motion')
```

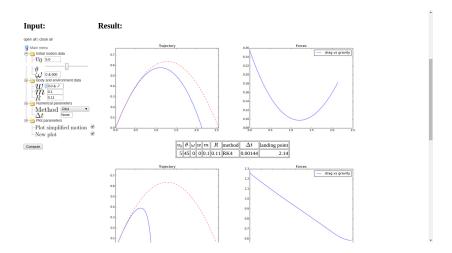


Figure 11: Web interface with documentation, LATEX symbols, and multiple input values.

Note that we accumulate the HTML code returned from the compute_motion_and_forces function that runs the simulation and returns the results as HTML code. Figure 11 mathematical description of the application, LATEX symbols as parameter names, and two input values for two parameters, leading to $2 \times 2 = 4$ runs, and hence four lines of plots. One realizes how easy it is to quickly perform parameter studies by simply 1) writing the compute function with loops and menu.get_values, 2) separating input values by & in the GUI.

3.9 2DO

- Lorenz demo as exercise, provide the compute function and graphics, perhaps also good demo in web4sciapps.
- units and text fields: Done
- menu list: no doc
- menu API: add doc in doc.html, also show possibility to call

- Check if multiple answers are correctly handled in DataItem, make enable_multiple_answers(*args) which turns all widgets into textline (or those given as arguments), make multiple loop parameters, can get them as list of dicts menu.get_multiple_values(*args) (all if no argument, otherwise those params listed), let keys be either full path or shortest possible path, can iterate over this list, test in ball example by having a new function with the multiple loop calling up compute_motion_and_forces_plot with new_plot=True first time and false the next times.
- Let w be function, widget=texline, str2type can be StringFunction. Can
 also invent a special syntax and translate to StringFunction or just make a
 function.
- Let w be filename: upload a Python module with the w(t) function.
- Problem: non-unique data item names cause trouble for the model class since just name is used as static variable...
- Show auto edit of the HTML code, e.g., removing Input: and Result:, this is easier than freezing the files and manually editing them. Reason: if you add new data itmes or submenus to the menu, it is convenient to be able to regenerate the whole setup.

```
from parampool.generator.flask.generate_template import \
    run_doconce_on_text
doc = run_doconce_on_text(compute_function.__doc__)
```

3.10 Reading default values from command line or file

To be programmed: Insert menu = set_defaults_from_file(menu) after calling menu_function. Then call set_values_from_command_line(menu) to override from command line. At the end of the controller.py script, dump menu to file again with write_menufile(filename). (The filename is given on the command line: --menufile filename.)

See the ...separate_submenus function - it has almost all this functionality!

3.11 Menu with other data structures

Filename and text field with special str2type conversion. Allow list syntax, but convert to array in str2type after list is eval'ed.

4 Advanced topics

This functionality much in place, but still not documented.

4.1 Login and archival of results

A user can create an account, log in, and save the results. The results of a run consists of the HTML code and plots, which are stored in a database. Later, old results can be retrieved in the GUI. Enabling login is just a matter of writing enable_login=True in the call to the generate function:

The generated controller.py file is now much more complicated in the Flask case, but the details are not important for the plain user of Parampool. The usage should be explanatory: first click on Register to register a new user, later one can just click on Login. After having run a similation, a Comments field arises where one can add comments about this run, and then click on Add if the results are sufficiently interesting to be stored in the database. The upper right corner has a link Previous simulations which gives access to previous results in the database. At the bottom of the page with previous runs, there is a Delete all button that clears the database.

4.2 Animations

4.3 Python expressions as input

This can only be done in menus unless the value of the parameter is a string (positional argument or default field as text, with explicit conversion). Treat menu only - drop implementation for inspection of compute function.

Describe input as

- sin(2.5)*exp(-1) (need to specify py code to be included in the controller/views or add such code manually? or do from numpy import * always? an argument with pycode is probably smart, the menu needs something similar for running str2type=eval in the right namespaces, could just be an additional data item attr namespace that, if present, is used if str2type is eval yes, that's the solution)
- MySpecialObject(2,3,4) (works)

5 Exercises

Exercise 1: Make a web app for integration

The purpose of this exercise is to use Parampool to generate a simple web application for integrating functions: $\int_a^b f(x)dx$. Provide a symbolic expression for f(x) and the limits a and b as input. The application returns the integral of

 $\int_a^b f(x)dx$ computed by some numerical integration rule (e.g., the Trapezoidal rule). Also try to integrate f(x) symbolically with the aid sympy and write out the anti-derivative of f(x) if the integration is successful.

Hint. The relevant sympy code needs to turn the string expression for f(x) into a valid symbolic expression via eval. This process requires import of the mathematical functions in sympy. Thereafter, the integrate functionality in sympy can be used to compute the integral.

```
def symbolic_integration(f_str):
    """
    Return the LaTeX code of the anti-derivative of f(x),
    where f_str holdes the formula for f(x) in a string.
    Return None if sympy cannot compute the anti-derivative.
    """
    from sympy import Symbol, integrate, \
        sin, cos, tan, log, asin, acos, atan, \
        sinh, cosh, tanh, asinh, acosh, atanh, erf, erfc,
    x = Symbol('x')
    f = eval(f_str)
    I = integrate(f, x)
    if isinstance(I, Integral):
        return None
    else:
        return latex(I)
```

6 Exercise: Make a web app for studying vibrations

Download bumpy. Set up prms.

$$mu'' + f(u') + s(u) = F(t),$$
 (4)

Make an interface to it such that

- s=k*u, have k as parameter, linear damping, F=0, V=0
- $F=A*\sin(w*t)$, A and w are parameters
- damping with two values and radio buttons, b
- s is a text expression
- F is a filename (0 is default)
- there is a submenu for F with different models: filename, A*sin(w*t) (submenu), white noise with intensity, formula of t
- another submenu for s models

On the main menu: damping can have radio buttons for linear b*u and quadratic b*u**2, F has list of different type of forces

Problem 2: Make a coin flipper

Make a web application where we can set the number of coins to be flipped. Clicking on the *Submit* button (whose name should rather be *flip*) shows images of coins with heads and tails according to a random flip of each coin.

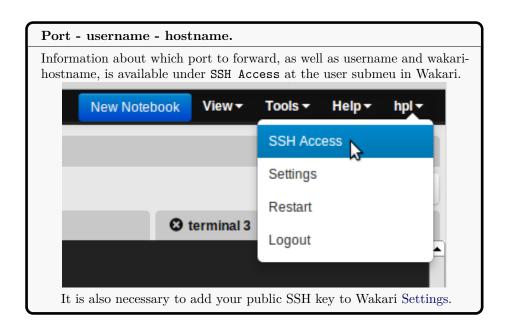
Hint. See random.org/coins for inspiration and images of coins. Filename: coin_flipper.

7 Deployment

The most obvious servers to deploy web applications on, like Google App Engine, only support very light weight Python. For heavier scientific applications we may need more tools; SSH access, a Fortran compiler, etc. Therefore we introduce two servers we recommend for the scientific computing usage.

7.1 Wakari

Wakari is originally meant to be a Python data analysis environment for internetaccessible services and sharing of computing environments. It does not allow users to deploy webservers that can be accessed by others. However, accessing a Flask server process running in Wakari is possible using SSH tunneling:



Now the application is available as usual at http://127.0.0.1:5000/ on your laptop.

Even though only Flask and not Django is pre-installed in Wakari, it is relatively straight-forward to download Django source and install it locally to your user. Also, if Gnuplot is to be installed and compiled with PNG support, the library Pnglib needs to be installed before Gnuplot is compiled.

7.2 Uni Oslo

The biggest downside with the Uni Oslo server is that you need to be a student or employee to access it. Nevertheless, the procedure described below for running web applications through a CGI script can be applied to any server.

If only little traffic has to be handled, it is possible to run Flask and Django through a CGI script. The script imports and starts the application's wsgi handler and works as a gateway between the Internet and the Flask or Django server.

The simplest example of a CGI script running Flask follows:

```
#!/usr/bin/python
from wsgiref.handlers import CGIHandler
from controller import app
CGIHandler().run(app)
```

This code assumes that the Python executive in /usr/bin/ is available and up-to-date, and that all required Python modules are on the PYTHONPATH environment and are available to be run by others. As the Python version on the Uni Oslo server, version 2.5, is no longer supported by the Python web frameworks, we need to install a newer version locally and use the absolute path to its executive in the header of the CGI script.

With a new Python installation we also need to (re)install all required modules and add them to sys.path. The script install_on_uio.sh in the top directory of cbc-websolver installs all required packages locally. Then we can add the location of these modules to sys.path in the CGI script:

```
import sys
sys.path += ['/path/to/local/installation/lib/python2.7/site-packages/']
CGIHandler().run(app)
```

One also needs to assure that the location of controller.py is in sys.path, or the import of app will fail.

The only difference between the CGI script for Flask and Django is that for Django one needs to add the directory containing the settings.py file to sys.path and set os.environ['DJANGO_SETTINGS_MODULE'] to settings. Also, the import of the app is a bit different than before:

```
sys.path += ['path/to/myproject'] # The folder containing settings.py
os.environ['DJANGO_SETTINGS_MODULE'] = 'myproject.settings'
app = django.core.handlers.wsgi.WSGIHandler()
CGIHandler().run(app)
```

Make CGI script accessible for others.

Remember that all scripts and modules to be accessed from the web need to have permissions for everyone to read and execute. This can be done by, e.g.,

Terminal > chmod 755 run_django.cgi

A Installation

We need

- Flask: sudo pip install Flask
- Django (optional): sudo pip install django
- $\bullet\ \mathrm{progressbar} \colon \mathtt{sudo}\ \mathtt{pip}\ \mathtt{install}\ \mathtt{progressbar}$
- ullet Flask-WTF: pip install Flask-WTF
- Flask-SQLAlchemy: sudo pip install Flask-SQLAlchemy
- Flask-Login: sudo pip install Flask-Login
- Flask-Mail: sudo pip install Flask-Mail
- Scientific Python for menu if units are used

Terminal> hg clone https://bitbucket.org/khinsen/scientificpython Terminal> cd scientificpython Terminal> sudo python setup.py install