# **PHYS Simulation API**

Release 1.0

Juan E. Aristizabal

# **GETTING STARTED**

Using PHYS Simulation API you can request simulations of some physical or mathematical systems such as the Harmonic Oscillator or the Chen-Lee Attractor –and soon many others, stay tuned!

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## **CHAPTER**

# **ONE**

# **HISTORY**

PHYS Simulation API started as a way of learning to develop an API. We believe that the best way of learning is by doing. This way, we chose a topic that drives us (yes, physics and mathematics!) and started learning by writting code! Of course, we had to read a lot and fail a lot as well, but we managed to develop our very first web application and we are proud of it, as impefect as it may be.

In the future we want to add as many features as we can, so far it enriches the client experience.

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#### **CHAPTER**

# **TWO**

# **GETTING STARTED**

# 2.1 Overview

In PHYS Simulation API you can request –via HTTP POST method– a simulation from a list of available simulations. Here we will show you the schemas you need to appropriately request your simulation. In *Examples* you will see how this works in the real life.

# 2.1.1 Request a simulation

 $The \ simulation \ requests \ are \ made \ in \ route \ / \verb|api/simulate/{sim\_system}|, \ where \ sim\_system \ is \ one \ of \ the \ members \ of \ SimSystem.$ 

The body of the request must abide by the following schema

## 2.1.1.1 SimRequest

Schema needed to request simulations via POST in /api/request/{sim_system}.					
type	object	object			
properties	·				
• system	SimSystem	SimSystem			
	type	string			
• t_span	T Span	T Span			
	type	array			
	default				

continues on next page

Table 1 – continued from previous page

	items	type	number			
• t_eval	T Eval					
	type	array				
	default					
	items	type	number			
• t_steps	T Steps	•				
	type	integer				
	default	0				
• ini_cndtn	Ini Cndtn					
	type	array				
	default					
	items	type	number			
• params	Params					
	type	object				
	additionalProperties	type	number			
• method	IntegrationMethods					
	type	string				
• username	Username					
	type	string				
	default	Pepito Perez				
definitions						
• SimSystem	SimSystem					
	List of available systems for simulation.					
	type	string				
	enum	Harmonic-Oscillator, Chen-Lee-Attractor				
<ul> <li>IntegrationMethods</li> </ul>	IntegrationMethods					
	List of available integration methods.					
	For more information see scipy.integrate.solve_ivp.					
	type	string				
	enum	RK45, RK23				

The body of the HTML response will have the following schema

## 2.1.1.2 SimIdResponse

Schema for the response of a simulation re	equest (requested via POST in route /api/simula	te/{sim_sys}.)		
type	object	object		
properties	·			
• sim_id	Sim Id			
	type	string		
• user_id	User Id	User Id		
	type	integer		
• username	Username			
	type	string		
• sim_sys	SimSystem			
	type	string		
• sim_status_path	Sim Status Path			
	type	string		
<ul><li>sim_pickle_path</li></ul>	Sim Pickle Path			
	type	string		
• message	Message			
	type	string		

# 2.1.2 Request Simulation Status

The response of the request simulation (SimIdResponse) contains a simulation ID, sim\_id. In order to know the simulation status you just need to make an HTTP request via GET with empty body in route /api/request/status/{sim\_id}.

**Note:** The route will be available just after the simulation is finished. If you do not receive a successful response and you are sure about the sim\_id you provided in the API route, the simulation may still be in course.

The schema of the response will be the following

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## 2.1.2.1 SimStatus

pe	object						
roperties							
• sim_id	Sim Id						
	type	string					
• user_id	User Id						
	type	integer					
• date	Date	•					
	type	string					
	format	date-time					
• system	SimSystem						
	type	string					
• ini_cndtn	Ini Cndtn						
	type	array					
	items	type	number				
• params	Params						
	type	object					
	additionalProperties	type	type number				
<ul> <li>method</li> </ul>	IntegrationMethods						
	type	string					
<ul> <li>route_pickle</li> </ul>	Route Pickle						
	type	string					
<ul><li>route_results</li></ul>	Route Results						
	type	string					
<ul> <li>route_plots</li> </ul>	Route Plots						
	type	string					
plot_query_values	PlotQueryValues						
	type	array					
	items	anyOf		PlotQueryValues_HO			
			type		object		
			additionalPro		type	S	tring
			PlotQuery	Values_C			
			type		object		

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# Table 2 – continued from previous page

		additionalProperties	type	string	
• plot_query_receipe	Plot Query Receipe				
	type	string			
	default	'route_plots' + '?value=' + 'plot_query_value'			
• success	Success				
	type	boolean			
<ul> <li>message</li> </ul>	Message				
	type	string			
definitions					
<ul> <li>SimSystem</li> </ul>	SimSystem				
	List of available systems for	r simulation.			
	type	string			
	enum	Harmonic-Oscillator, Chen-Lee-Attractor			
<ul> <li>IntegrationMethods</li> </ul>	IntegrationMethods				
	List of available integration methods.				
	For more information see scipy.integrate.solve_ivp.				
	type	string			
	enum	RK45, RK23			
•	PlotQueryValues_HO				
PlotQueryValues_HC	List of tags of each different plot generated automatically by the				
	backend when a Harmonic Oscillator simulation is requested.				
	type	string			
	enum	coord, phase			
•	PlotQueryValues_ChenLee				
PlotQueryValues_Ch		t plot generated automatically by the			
	backend when a Chen-Lee simulation is requested.				
	type	string			
	enum	threeD, project			

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## 2.1.3 Request Results

If success=True in SimStatus, you can

- 1. Directly download your results
  - a. Download pickle file with all the simulation results as returned by scipy.integrate.solve\_ivp. You can do this via GET with empty body in route /api/results/{sim\_id}/pickle.
  - b. Download your simulation's automatically generated plots. You can do this via GET with empty body in route /api/results/{sim\_id}/plot? value={plot\_query\_value}, where plot\_query\_value is one of the items in plot\_query\_values in the simulation status, SimStatus.
- 2. See your results online. You can do this via GET in route /results/{sim\_system}/{sim\_id}. In the rendered HTML file, you have the option to download both the generated plots and the pickle file mentioned in the last item.

# 2.2 Examples

Here we will see an example of the work flow with PHYS Simulation API. To make HTTP requests we will use the requests Python library.

Let's see our API in action!

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## 2.2.1 1. Request Simulation

Lets start with some imports and defining our simulation request body.

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```
>>>
        "t_span": [0, 200],
        "t_steps": 1e5,
>>>
        "ini_cndtn": [10, 10, 0],
>>>
        "params": {
>>>
           "a": 3,
>>>
            "b": -5,
>>>
            "c": -1,
>>>
>>>
>>> }
```

Note that sim\_request follows the pydantic model simulation\_API.controller.schemas.SimRequest. For the ChenLeeAttractor, the initial condition array is of length 3, and the parameters are a, b and c. In your case, the conditions may be different, so you must check what are the parameters and what are the initial conditions for the system you want to simulate.

Now we request the simulation via post to the appropriate route and print the result

```
>>> # PHYS Simulatio URI
>>> url = 'http://0.0.0.0:5700'
>>>
>>> # Simulation request route
>>> sim_requrest_route = f'/api/simulate/{sim_system}'
>>>
>>> # Request simulation via HTTP using `requests` module
>>> sim_request_response = requests.post(url + sim_requrest_route, json=sim_request)
>>>
>>> # Print response
>>> print(
>>>
        "Simulation Request Response",
>>>
>>>
        f"HTML status code: {sim_request_response.status_code}",
>>>
        "Response:",
>>>
        " { ",
>>>
>>>
        sep='\n',
>>> )
>>> for key, v in sim_request_response.json().items():
                       '{key}': {v}")
        print(f"
>>>
>>> print(" }")
```

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We have just finished the first step in the workflow. We now know our sim\_id how to request the simulation results.

## 2.2.2 2. Request Simulation Status

We proceed now to request the simulation results via GET in route /api/simulate/status/{sim\_id}.

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```
>>> print(
>>>
>>>
        "Simulation status Response",
       "_____",
>>>
       f"HTML status code: {sim_status_response.status_code}",
>>>
       "Response:",
>>>
       " { ",
>>>
       sep=' \n',
>>>
>>> )
>>> for key, v in sim_status_response_json.items():
                     '{key}': {v},")
       print(f"
>>> print(" }\n")
Simulation status Response
HTML status code: 200
Response:
        'sim_id': e5f6d0e0719b45fea4aa9f098e12e7c3,
        'user_id': 1,
        'date': 2020-10-05T23:31:24.977484,
        'system': Chen-Lee-Attractor,
        'ini_cndtn': [10.0, 10.0, 0.0],
        'params': {'a': 3.0, 'b': -5.0, 'c': -1.0},
        'method': RK45,
        'route_pickle': /api/results/e5f6d0e0719b45fea4aa9f098e12e7c3/pickle,
        'route_results': /api/simulate/status/e5f6d0e0719b45fea4aa9f098e12e7c3,
        'route_plots': /api/results/e5f6d0e0719b45fea4aa9f098e12e7c3/plot,
        'plot_query_values': ['threeD', 'project'],
        'plot_query_receipe': 'route_plots' + '?value=' + 'plot_query_value',
        'success': True,
        'message': Finished. You can request via GET: download simulation results (pickle) in route given in 'route_pickle', or;
→download plots of simulation in route 'route_plots' using query params the ones given in 'plot_query_values', or; see results.
→online in route 'route results'.,
```

Note the sleep (5) call at the beginning of this code block. We did this in order to be sure that the simulation was completed. If we request the simulation status too soon, it may not be available and an appropriate message will be returned in the response as well as "success": False.

Also note that in the "message" it is clearly stated how to access the results.

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## 2.2.3 3. Request Simulation Results

Now we proceed to download the pickle and the plots, as stated in the simulation status "message".

Lets start with the pickle

```
>>>
>>> if not sim_status_response_json["success"]:
       print("Warning: pickle and plot files not available.\n")
>>>
>>>
       sys.exit(1)
>>>
>>> # Pickle download route
>>> pickle_route = sim_status_response.json()["route_pickle"]
>>>
>>> # Request simulation status via HTTP using `requests` module
>>> pickle_response = requests.get(url + pickle_route, stream=True)
>>>
>>> # Get our directory absolute path
>>> this_directory = os.path.dirname(__file__)
>>>
>>> # Save Pickle
>>> with open(this_directory + '/simulation.pickle', 'wb') as file:
       file.write(pickle_response.content)
```

The generated file is named simulation.pickle and contains all the information of the simulation results.

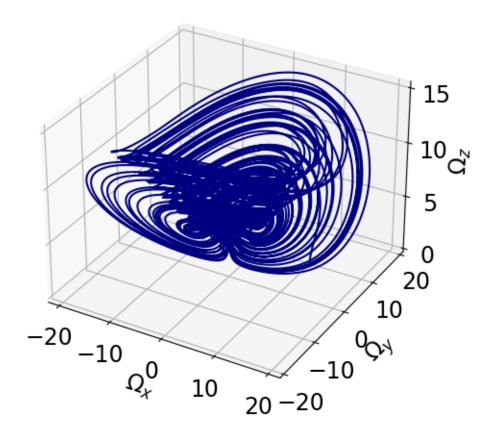
Finally, lets download the plots

```
>>> # Plots download route
>>> plots_route = sim_status_response.json()["route_plots"]
>>>
>>> # Plot query values
>>> plot_query_values = sim_status_response.json()["plot_query_values"]
>>>
>>> for qv in plot_query_values:
        # Construct the URI query for each plot
>>>
        plot_query_url = url + plots_route + "?value=" + qv
>>>
>>>
        # Request the plot
>>>
        plot_response = requests.get(plot_query_url, stream=True)
>>>
```

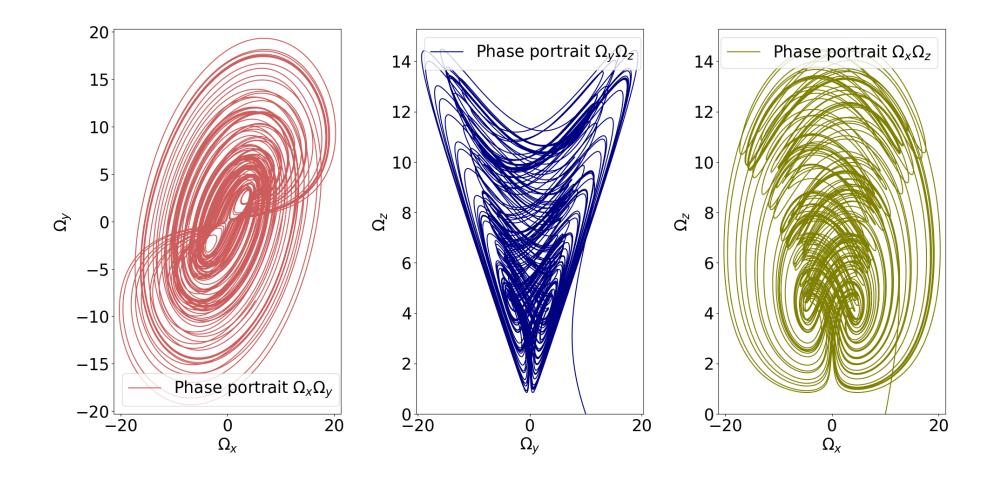
(continues on next page)

```
>>>
>>>
    # Save the plot in a file
>>>    plot_file_name = this_directory + "/plot_" + qv + ".png"
>>>    with open(plot_file_name, 'wb') as file:
>>>    file.write(plot_response.content)
```

The two generated plots are named plot\_threeD.png and plot\_project.png and are respectively displayed below.



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# 2.3 Website

This API has a very simple website, where you can request your simulations and see all the available results, as well as some pretty plots of each simulation.

The website, called PHYS Simulation is self-explanatory. Just dive in and request your simulations!

- Overview
- Examples
- Website

2.3. Website

**CHAPTER** 

**THREE** 

# **FOR DEVELOPERS**

This API is built on top of FastAPI. If you want to contribute to this project, you may find their docs very useful.

In this section you can find all the source code docuentation. If you have a question on how some function, class or method works, maybe it's answered here. If not, do not hesitate to contact us.

# 3.1 The Code

# 3.1.1 simulation\_api Package

# 3.1.1.1 Package contents

This module initializes our application.

## 3.1.1.2 Subpackages

3.1.1.2.1 simulation api.controller

#### 3.1.1.2.1.1 Package contents

#### 3.1.1.2.1.2 Submodules

#### 3.1.1.2.1.3 simulation\_api.controller.main

This file manages all requests that are made to our app

**Parameters**  $sim_id(str)$  – ID of the simulation.

**Returns** FileResponse containing the simulation results in pickle format.

**Return type** starlette.responses.FileResponse

Download plot of previously requested simulation.

Note one query param is required here.

Here we use FileResponse from starlette.responses

#### **Parameters**

- $sim_id(str)$  ID of the simulation.
- value (PlotQueryValues) Query values. Must be a member of one of the Enum classes given in PlotQueryValues.

**Returns** FileResponse containing the requested plot.

 $\textbf{Return type} \ \ \text{starlette.responses.} File Response$ 

async simulation\_api.controller.main.api\_simulate\_sim\_system ( $sim_system$ : simulation\_api.controller.schemas.SimSystem,  $sim_params$ : simulation\_api.controller.schemas.SimRequest,  $background_tasks$ :  $star-lette.background_tasks$ , db:  $sqlalchemy.orm.session.Session = Depends(get_db)) o simulation_api.controller.schemas.SimIdResponse$ 

In this route the client can request a simulation.

When the client requests a simulation via /api/simulate/{sim\_system}, he/she obtains relevant information on how to get the results of the simulation.

Note: Here we use fastapi.BackgroudTasks to make the simulation in the background.

#### **Parameters**

- sim\_system (SimSystem) System to be simulated.
- sim\_params (SimRequest) Simulation request information with schema given by SimRequest and decalared in schemas.py.
- background\_tasks (BackgroundTasks) Background task FastAPI manager (Class). This is handled internally.
- **db** (Session) Database Session, needed to interact with database. This is handled internally.

**Returns** sim\_id\_response – Contains relevant information about the simulation and how to get the results.

Return type SimIdResponse

```
async simulation_api.controller.main.api_simulate_status_sim_id (sim_id: str, db: sqlalchemy.orm.session.Session = Depends(<math>get_idb)) \rightarrow simulation_api.controller.schemas.SimStatus

Obtains status of requested simulation.
```

#### **Parameters**

•  $sim_id(str)$  – ID of the simulation.

Starts and ends session in each route that needs database access

• **db** (Session) – Database Session, needed to interact with database. This is handled internally.

**Returns** Status information of the simulation and how to get the results.

## **Return type** SimStatus

```
async simulation_api.controller.main.custom_http_exception_handler(request: starlette.requests.Request, exc: starlette.exceptions.HTTPException)

Handles 404 exceptions by rendering a template.

simulation api.controller.main.get db()
```

```
async simulation_api.controller.main.index (request: starlette.requests.Request)
Index frontend web page.
```

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**Parameters** request (Request) – HTTP request, used internally by FastAPI.

**Returns** Renders greeting template and hyperlinks to simulation rquests and results.

Return type fastapi.templating.Jinja2Templates.TemplateResponse

**async** simulation\_api.controller.main.results (request: starlette.requests.Request, db: sqlalchemy.orm.session.Session = Depends(get\_db))

Renders web page showing a list of all the available simulation results.

#### **Parameters**

- request (Request) HTTP request, used internally by FastAPI.
- db (Session) Database Session, needed to interact with database. This is handled internally.

**Returns** Template displaying all the available simulation results.

Return type fastapi.templating.Jinja2Templates.TemplateResponse

async simulation\_api.controller.main.results\_sim\_system\_sim\_id(request: starlette.requests.Request, sim\_system: simulation\_api.controller.schemas.SimSystem, sim\_id: str)

Shows graphic results of a simulation in frontend for a given sim\_id.

#### **Parameters**

- request (Request) HTTP request, used internally by FastAPI.
- sim\_system (SimSystem) System to be simulated.
- $sim_id(str)$  ID of the simulation.

**Returns** Template displaying all the generated plots for a given simulation.

Return type fastapi.templating.Jinja2Templates.TemplateResponse

async simulation\_api.controller.main.simulate(request: starlette.requests.Request)
 Simulate web page.

Here the clients can select between the available systems to simulate their preferred one.

**Parameters** request (Request) – HTTP request, used internally by FastAPI.

**Returns** Template displaying the available systems to be simulated.

 $\textbf{Return type} \ \texttt{fastapi.templating.Jinja2Templates.TemplateResponse}$ 

**async** simulation\_api.controller.main.simulate\_id\_sim\_id(request: starlette.requests.Request, sim\_id: str)
Shows simulation id after asking for simulation in frontend form.

#### **Parameters**

- request (Request) HTTP request, used internally by FastAPI.
- $sim_id(str)$  ID of the simulation.

**Returns** Template displaying the simulation ID and a hyperlink to further information about the simulation.

Return type fastapi.templating.Jinja2Templates.TemplateResponse

```
async simulation_api.controller.main.simulate_sim_system(request: starlette.requests.Request, sim_system: simulation_api.controller.schemas.SimSystem, error_message: Optional[str] = ")
Simulation's form web page.
```

The clients input the desired parameters for the simulation of their choosing.

#### **Parameters**

- request (Request) HTTP request, used internally by FastAPI.
- sim system (SimSystem) System to be simulated.
- error\_message (str) Internally used by the backend to display error messages in forntend form.

**Returns** Template displaying the simulation request form.

 $\textbf{Return type} \ \texttt{fastapi.templating.Jinja2Templates.TemplateResponse}$ 

```
async simulation_api.controller.main.simulate_sim_system_post(request:
                                                                                               starlette.requests.Request,
                                                                                                                          sim_system:
                                                                                                                                            simula-
                                                                                tion_api.controller.schemas.SimSystem,
                                                                                                                       background_tasks:
                                                                                                                                               star-
                                                                                lette.background.BackgroundTasks, db: sqlalchemy.orm.session.Session =
                                                                                Depends(get_db), sim_sys: simulation_api.controller.schemas.SimSystem
                                                                                 = Form(Ellipsis), username:
                                                                                                                str = Form(Ellipsis), t0:
                                                                                                                                              float
                                                                                 = Form(Ellipsis), tf:
                                                                                                          float = Form(Ellipsis), dt:
                                                                                                                                           float =
                                                                                                          int = Form(Ellipsis), method:
                                                                                Form(Ellipsis), t steps:
                                                                                                                                            simula-
                                                                                tion api.controller.schemas.IntegrationMethods = Form(Ellipsis))
```

Receives the simulation request information from the frontend form and requests the simulation to the backend.

This route receives the form requesting a simulation (filled in frontend via GET in route /simulate/{sim\_system}). The simulation is internally requested using the function <code>simulation\_api.controller.tasks.\_api\_simulation\_request()</code>. Finally the client is redirected to the "Simulation ID" frontend web page, where further information about the simulation is displayed.

#### **Parameters**

• request (Request) – HTTP request, used internally by FastAPI.

3.1. The Code

- **sim\_system** (SimSystem) System to be simulated.
- background tasks (BackgroundTasks) Needed to request simulation to the backend (in background). Handled internally by the API.
- db (Session) Database Session, needed to interact with database. This is handled internally.
- sim\_sys (SimSystem) Form entry: system to be simulated. Must be one of the members of SimSystem.
- **username** (str) Form entry: name of the user requesting the simulation.
- **t0** (*float*) Form entry: initial time of simulation.
- **tf** (*float*) Form entry: final time of simulation.
- **dt** (*float*) Form entry: timestep of simulation.
- t\_steps Form entry: number of time steps. If different from 0 or None, dt is ignored.
- method (IntegrationMethods) Form entry: method of integration. Must be a member of IntegrationMethods.

**Returns** If the client made a mistake filling the form renders the simulation request form again. Otherwise, redirects the client to "Simulation ID" frontend web page.

Return type fastapi.templating.Jinja2Templates.TemplateResponse or starlette.responses.RedirectResponse

**Note:** The values of the form accessed by fastapi.Form are only declared as parameters so that pydantic checks the types, but they are not used directly to request the simulation. Here, we access the form directly by using the method fastapi.Request.form() as can be seen in the first lines of this function. This allows us a better control over the data and also to handle different type of forms—which depend on the simulation because parameters and initial conditions are intrinsically different for different systems.

#### **Parameters**

- request (Request) HTTP request, used internally by FastAPI.
- $sim_id(str)$  ID of the simulation.
- **db** (Session) Database Session, needed to interact with database. This is handled internally.

**Returns** Template displaying the simulation status and a hyperlinks to simulation results in several formats. If simulation id is not available (not yet in database), renders a message about the situation.

Return type fastapi.templating.Jinja2Templates.TemplateResponse

#### 3.1.1.2.1.4 simulation api.controller.schemas

This module defines all the models/schemas needed in our application, except the database models required for sqlalchemy ORM.

class simulation\_api.controller.schemas.ChenLeeParams (\*, a: float, b: float, c: float)
 Bases: pydantic.main.BaseModel

List of parameters of the Chen-Lee Attractor system.

**Note:** For more information about Chen-Lee Attactor's parameters see ChenLeeAttractor.

Warning: This needs update each time a new simulation is added: add an appropriate new class similar to this one or to HOParams.

a: float

 $\omega_x$  parameter.

b: float

 $\omega_y$  parameter.

c: float

 $\omega_z$  parameter.

class simulation\_api.controller.schemas.ChenLeeSimForm (\*, username: str = 'Pepito', t0: float = 0.0, tf: float = 6.283185307179586, dt: float = 0.3141592653589793,  $t\_steps$ : int = 0, method:  $simulation\_api.controller.schemas.IntegrationMethods = 'RK45'$ ,  $sim\_sys$ :  $simulation\_api.controller.schemas.SimSystem = 'Chen-Lee-Attractor', <math>ini0$ : float = 10.0, ini1: float = 10.0, ini2: float = 0.0, param0: float = 3.0, param1: float = -5.0, param2: float = -1.0)

Bases: simulation\_api.controller.schemas.SimForm

Schema used to Request Chen Lee Simulation in Frontend via form.

**Note:** For more information about Chen-Lee Attactor simulation see ChenLeeAttractor.

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ini0: Optional[float]

 $\omega_x$  initial condition.

ini1: Optional[float]

 $\omega_y$  initial condition.

ini2: Optional[float]

 $\omega_z$  initial condition.

param0: Optional[float]

Parameter of name ChenLeeParams.a.

param1: Optional[float]

Parameter of name ChenLeeParams.b.

param2: Optional[float]

Parameter of name ChenLeeParams.c.

sim\_sys: simulation\_api.controller.schemas.SimSystem

System to be simulated.

class simulation\_api.controller.schemas.HOParams(\*, m: float, k: float)

Bases: pydantic.main.BaseModel

List of parameters of the Harmonic Oscillator system.

Note: For more information about Harmonic Oscillator's parameters see <code>HarmonicOsc1D</code>.

Warning: This needs update each time a new simulation is added: add an appropriate new class similar to this one or to ChenLeeParams.

k: float

Force constant of object.

m: float

Mass of object.

```
class simulation_api.controller.schemas.\texttt{HOSimForm}(*, username: str = 'Pepito', t0: float = 0.0, tf: float = 6.283185307179586, dt: float = 0.3141592653589793, t_steps: int = 0, method: simulation_api.controller.schemas.IntegrationMethods = 'RK45', sim_sys: simulation_api.controller.schemas.SimSystem = 'Harmonic-Oscillator', ini0: float = 1.0, ini1: float = 0.0, param0: float = 1.0, param1: float = 1.0)

Bases: simulation_api.controller.schemas.SimForm

Schema used to Request Harmonic Oscillator Simulation in Frontend via form.
```

Note: For more information about Chen-Lee Attactor simulation see HarmonicOsc1D.

```
ini0: Optional[float]
   q initial value.
```

ini1: Optional[float]
 p initial value.

param0: Optional[float]
 Parameter of name HOParams.m.

param1: Optional[float]
 Parameter of name HOParams.k.

sim\_sys: simulation\_api.controller.schemas.SimSystem
System to be simulated.

 $\textbf{class} \texttt{ simulation\_api.controller.schemas.IntegrationMethods} \ (\textit{value})$ 

Bases: str.enum.Enum

List of available integration methods

**Note:** For more information about these integration methods see scipy.integrate.solve\_ivp.

**Warning:** Please update this class with relvant simulation methods available in scipy.integrate.solve\_ivp –only the ones that do not require more parameters than the ones provided in SimRequest.

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RK23 = 'RK23'

```
Explicit Runge-Kutta method of order 3(2).
     RK45 = 'RK45'
         Explicit Runge-Kutta method of order 5(4).
class simulation_api.controller.schemas.IntegrationMethodsFrontend(value)
     Bases: str.enum.Enum
     List of captions of available integration methods. These are displayed in frontend simulation form.
      Warning: This class needs update each time a new simulation is added: add an appropriate new attribute.
     RK23 = 'Runge-Kutta 3(2)'
     RK45 = 'Runge-Kutta 5(4)'
class simulation api.controller.schemas.ParamType (value)
     Bases: str, enum. Enum
     These are the possible values of param_type column in parameters table in simulations.db database.
     ini cndtn = 'initial condition'
     param = 'parameter'
class simulation_api.controller.schemas.ParameterDBSch(*, sim_id: str = None, param_type: simulation_api.controller.schemas.ParamType
                                                                    = None, param_key: str = None, ini_cndtn_id: int = None, value: float = None,
                                                                    param id: int = None
     Bases: simulation_api.controller.schemas.ParameterDBSchBase
     Model for API type checking when reading a row in parameters table in simulations.db database.
     class Config
         Bases: object
         This class is needed for database reading optimization (thanks to Object Relational Mapper -ORM.)
         Note: Read more in FastAPI docs.
         orm model = True
```

```
param_id: Optional[int]
class simulation api.controller.schemas.ParameterDBSchBase(*,
                                                                            sim id:
                                                                                                     None.
                                                                                                                                simula-
                                                                                                              param type:
                                                                      tion_api.controller.schemas.ParamType = None, param_key: str = None,
                                                                      ini \ cndtn \ id: int = None, value: float = None)
    Bases: pydantic.main.BaseModel
    Basemodel for API type checking when querrying parameters table in simulations. db database.
    ini_cndtn_id: Optional[int]
    param_key: Optional[str]
    param_type: Optional[simulation_api.controller.schemas.ParamType]
    sim_id: Optional[str]
    value: Optional[float]
class simulation_api.controller.schemas.ParameterDBSchCreate (*, sim_id: str, param_type: simulation_api.controller.schemas.ParamType,
                                                                        param key: str = None, ini cndtn id: int = None, value: float)
    Bases: simulation api.controller.schemas.ParameterDBSchBase
    Model for API type checking when creating a row in parameters table in simulations.db database.
    param_type: simulation_api.controller.schemas.ParamType
    sim id: str
    value: float
class simulation_api.controller.schemas.PlotDBSch(*, sim_id: str = None, plot_query_value: str = None, plot_id: int = None)
    Bases: simulation_api.controller.schemas.PlotDBSchBase
    Model for API type checking when reading a row in plots table in simulations.db database.
    class Config
         Bases: object
         This class is needed for database reading optimization (thanks to Object Relational Mapper –ORM.)
         Note: Read more in FastAPI docs.
```

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orm model = True

```
plot_id: Optional[int]
class simulation api.controller.schemas.PlotDBSchBase(*, sim id: str = None, plot query value: str = None)
     Bases: pydantic.main.BaseModel
     Basemodel for API type checking when querrying plots table in simulations.db database.
    plot_query_value: Optional[str]
     sim id: Optional[str]
class simulation api.controller.schemas.PlotDBSchCreate(*, sim id: str, plot query value: str)
     Bases: simulation api.controller.schemas.PlotDBSchBase
    Model for API type checking when creating a 'plot information' row in plots table in simulations.db database.
    plot_query_value: str
     sim id: str
simulation_api.controller.schemas.PlotQueryValues = typing.Union[simulation_api.controller.schemas.PlotQueryValues_HO, simulation_
    Union of the classes defining Enums of plot query values for each system. This is needed in SimStatus.
class simulation_api.controller.schemas.PlotQueryValues_ChenLee(value)
     Bases: str.enum.Enum
    List of tags of each different plot generated automatically by the backend when a Chen-Lee simulation is requested.
    These tags are used as the possible values of the querry param value in route /api/results/{sim id}/plot?value=<plot query value>.
    Note: simualtion_API.controller.schemas.SimIdResponse.sim_id must be related to the Chen Lee system.
```

```
project = 'project'
threeD = 'threeD'
class simulation_api.controller.schemas.PlotQueryValues_HO(value)
    Bases: str, enum.Enum
```

List of tags of each different plot generated automatically by the backend when a Harmonic Oscillator simulation is requested.

These tags are used as the possible values of the querry param value in route /api/results/{sim\_id}/plot?value=<plot\_query\_value>.

```
Note: simualtion_API.controller.shcemas.SimIdResponse.sim_id must be related to the Harmonic Oscillator system.

coord = 'coord'

phase = 'phase'

class simulation_api.controller.schemas.SimForm(*, username: str = 'Pepito', t0: float = 0.0, tf: float = 6.283185307179586,

dt: float = 0.3141592653589793, t_steps: int = 0, method: simulation_api.controller.schemas.IntegrationMethods = 'RK45')

Bases: pydantic.main.BaseModel
```

Warning: Needs update each time a new simulation is added:

Basemodel of schema used to Request a Simulation in Frontend.

- 1. Create a new appropriate class similar to HOSimForm or to ChenLeeSimForm.
- 2. Add the class to the dict SimFormDict defined somewhere in this module.

## dt: Optional[float]

Time step size of simulation.

## method: Optional[simulation\_api.controller.schemas.IntegrationMethods]

Integration method used in simulation.

#### t0: Optional[float]

Initial time of simulation.

#### t steps: Optional[int]

Number of time steps. If different from 0, dt is ignored.

#### tf: Optional[float]

Final time of simulation.

#### username: Optional[str]

simulation\_api.controller.schemas.SimFormDict = {'Chen-Lee-Attractor': <class 'simulation\_api.controller.schemas.ChenLeeSimForm' Maps the name of each available system to its simulation form model.

3.1. The Code

Warning: Needs update each time a new simulation is added: add a new appropriate item to this dict.

```
class simulation api.controller.schemas. SimIdResponse (*, sim id: str = None, user id: int = None, username: str = None, sim sys:
                                                                    simulation api.controller.schemas.SimSystem = None, sim status path: str = None,
                                                                    sim\_pickle\_path: str = None, message: str = None)
     Bases: pydantic.main.BaseModel
     Schema for the response of a simulation request (requested via POST in route /api/simulate/{sim_sys}.)
     Note: The request of the simulation must follow the model SimRequest.
     message: Optional[str]
```

## Explanatory message.

#### sim\_id: Optional[str]

ID of simulation.

## sim\_pickle\_path: Optional[str]

Path to GET (download) a pickle with the results of the simulation.

### sim\_status\_path: Optional[str]

Path to GET the status of the simulation.

## sim\_sys: Optional[simulation\_api.controller.schemas.SimSystem]

Simulated system.

#### user\_id: Optional[int]

User id number stored in database.

username: Optional[str]

```
class simulation api.controller.schemas.SimRequest(*, system: simulation api.controller.schemas.SimSystem.HO: 'Harmonic-
                                                               Oscillator'>, t\_span: List[float] = [], t\_eval: List[float] = [], t\_steps: int
                                                               = 0, ini_cndtn: List[float] = [], params: Dict[str, float], method: simula-
                                                               tion api.controller.schemas.IntegrationMethods = 'RK45', sim id: str = None, user id: int
                                                               = 0, username: str = 'Pepito Perez')
```

Bases: pydantic.main.BaseModel

Schema needed to request simulations via POST in /api/request/{sim\_system}.

For the attributes that do not have a description see simulation\_api.simulation.simulations.Simulation.

**Note:** Most of the attributes in this pydantic class are arguments of the classes defined in the module simulation\_api.simulation.simulations, for more information please refer to It.

```
ini cndtn: List[float]
     method: Optional[simulation api.controller.schemas.IntegrationMethods]
     params: Dict[str, float]
     sim id: Optional[str]
         ID of simulation. This is handled internally, leave it blank when requesting a simulation.
               simulation_api.controller.schemas.SimSystem
     t_eval: Optional[List[float]]
     t span: List[float]
     t_steps: Optional[int]
     user_id: Optional[int]
         User id number stored in database. This is handled internally, leave it blank when requesting a simulation.
     username: str
class simulation api.controller.schemas.SimResults(*, sim results: scipy.integrate. ivp.ivp.OdeResult)
     Bases: pydantic.main.BaseModel
     Results of simulation as returned by scipy.integrate.solve ivp
     sim results: scipy.integrate. ivp.ivp.OdeResult
                                                                                                        datetime.datetime, system:
class simulation api.controller.schemas.SimStatus(*, sim id:
                                                                           str, user id:
                                                                                           int, date:
                                                             tion_api.controller.schemas.SimSystem = None, ini_cndtn: List[float] = None, params:
                                                             Dict[str, float] = None, method: simulation_api.controller.schemas.IntegrationMethods
                                                             = None, route_pickle: str = None, route_results: str = None, route_plots: str = None,
                                                                                List[Union[simulation_api.controller.schemas.PlotQueryValues_HO,
                                                             plot_query_values:
                                                             simulation_api.controller.schemas.PlotQueryValues_ChenLee]] = None, plot_query_receipe:
                                                             str = "'route\_plots' + '?value=' + 'plot\_query\_value'", success: bool = None, message: str =
                                                             None)
     Bases: pydantic.main.BaseModel
```

Schema of the status of simulations.

This pydantic model is intended to store paths of results of the simulations algong with some metadata. This information can be accessed via GET in /api/simulate/status/{sim\_id}.

date: datetime.datetime

Date of request of simulation.

ini\_cndtn: Optional[List[float]]

message: Optional[str]

Additional information on status of simulation.

method: Optional[simulation\_api.controller.schemas.IntegrationMethods]

params: Optional[Dict[str, float]]

plot\_query\_receipe: Optional[str]

plot\_query\_values: Optional[List[Union[simulation\_api.controller.schemas.PlotQueryValues\_HO, simulation\_api.controller.schemas.PlotQueryValues\_HO, simulatio

Query params values of different automatically generated plots. These values are needed to download the plots in route /api/results/{sim\_id}/plot? value=<plot\_query\_value>.

route\_pickle: Optional[str]

Route of pickle file generated by the simulation.

route plots: Optional[str]

Route of plots generated by the simulation backend.

route\_results: Optional[str]

Route of frontend showing results.

sim id: str

ID of simulation.

success: Optional[bool]

Success status of simulation.

system: Optional[simulation\_api.controller.schemas.SimSystem]

Simulated system.

user id: int

User id number stored in database.

 $\textbf{class} \texttt{ simulation\_api.controller.schemas.SimSystem} \ (\textit{value})$ 

Bases: str, enum. Enum

List of available systems for simulation.

**Warning:** The values of the attributes of this class must coincide with the dictionary keys defined in simulation\_api.simulations.simulations. Simulations, otherwise the system won't be simulated by the backend.

Warning: This class needs update each time a new simulation is added: add an appropriate new attribute.

ChenLee: str = 'Chen-Lee-Attractor'

Chen-Lee Attractor Enum attribute.

HO: str = 'Harmonic-Oscillator'

Harmonic Oscillator Enum attribute.

simulation\_api.controller.schemas.SimSystem\_to\_SimParams = {'Chen-Lee-Attractor': <class 'simulation\_api.controller.schemas.Chemas.Chemas.Chemas.chem

Warning: Needs update each time a new simulation is added: add a new appropriate item to this dict.

class simulation\_api.controller.schemas.SimulationDBSch (\*,  $sim\_id$ : str = None,  $user\_id$ : int = None, date: str = None, system: str = None,  $route\_pickle$ : str = None,

 $Bases: \verb|simulation_api.controller.schemas.SimulationDBSchBase|$ 

 $Model \ for \ API \ type \ checking \ when \ reading \ a \ row \ in \ \texttt{simulations} \ table \ in \ \texttt{simulations}. \ db \ database.$ 

class Config

Bases: object

 $This\ class\ is\ needed\ for\ database\ reading\ optimization\ (thanks\ to\ Object\ Relational\ Mapper\ -ORM.)$ 

**Note:** Read more in FastAPI docs.

```
orm model = True
    date: Optional[str]
    message: Optional[str]
    method: Optional[str]
    route_pickle: Optional[str]
    route_plots: Optional[str]
    route_results: Optional[str]
    sim_id: Optional[str]
    success: Optional[bool]
    system: Optional[str]
    user_id: Optional[int]
class simulation_api.controller.schemas.SimulationDBSchBase(*, sim_id: str = None, user_id: int = None, date: str = None, system: str =
                                                                  None, method: str = None, route\_pickle: str = None, route\_results: str = None,
                                                                  route\_plots: str = None, success: bool = None, message: str = None)
    Bases: pydantic.main.BaseModel
    Basemodel for API type checking when querrying simulations table in simulations.db database.
    date: Optional[str]
    message: Optional[str]
    method: Optional[str]
    route_pickle: Optional[str]
    route_plots: Optional[str]
    route_results: Optional[str]
    sim_id: Optional[str]
    success: Optional[bool]
    system: Optional[str]
    user_id: Optional[int]
```

```
class simulation_api.controller.schemas.SimulationDBSchCreate(*, sim_id: str, user_id: int, date: str, system: str, method: str = None,
                                                                            route\_pickle: str = None, route\_results: str = None, route\_plots: str = None,
                                                                            success: bool, message: str = None)
     Bases: simulation api.controller.schemas.SimulationDBSchBase
     Model for API type checking when creating a 'simulation information' row in simulations table in simulations. db database.
     date: str
     sim id: str
     success: bool
     system: str
     user_id: int
class simulation_api.controller.schemas.UserDBSch(*, username: str = None, user_id: int = None)
     Bases: simulation_api.controller.schemas.UserDBSchBase
    Model for API type checking when reading a user information in users table in simulations.db database.
     class Config
         Bases: object
         This class is needed for database reading optimization (thanks to Object Relational Mapper –ORM.)
         Note: Read more in FastAPI docs.
         orm model = True
     user_id: Optional[int]
class simulation_api.controller.schemas.UserDBSchBase(*, username: str = None)
     Bases: pydantic.main.BaseModel
     Basemodel for API type checking when querrying users table in simulations.db database.
     username: Optional[str]
class simulation_api.controller.schemas.UserDBSchCreate(*, username: str, hash_value: str = None)
     Bases: pydantic.main.BaseModel
     Model for API type checking when creating a 'user information' row in users table in simulations.db database.
```

```
hash_value: Optional[str]
    username: str

simulation_api.controller.schemas.params_mapping_ChenLee = {'param0': 'a', 'param1': 'b', 'param2': 'c'}
    Maps the name of each Chen-Lee Attractor parameter in frontend form to its name in backend (defined by its corresponding attribute in class ChenLeeAttractor)

simulation_api.controller.schemas.params_mapping_HO = {'param0': 'm', 'param1': 'k'}
    Maps the name of each Harmonic Oscillator parameter in frontend form to its name in backend (defined by its corresponding attribute in class HarmonicOsc1D)

simulation_api.controller.schemas.system_to_params_dict = {'Chen-Lee-Attractor': {'param0': 'a', 'param1': 'b', 'param2': Maps the name of each available system to its parameter change-of-convention mapping (e.g. params_mapping_HO or params_mapping_ChenLee.)

This is used to translate the parameters name convention in frontend simulation request to the parameters name convention in backend simulation request (with appropriate)
```

## 3.1.1.2.1.5 simulation api.controller.tasks

This file will do background tasks e.g. the simulation

schema given by SimRequest.)

```
simulation\_api.controller.tasks.\_api\_simulation\_request \ (sim\_system: simulation\_api.controller.schemas.SimSystem, sim\_params: simulation\_api.controller.schemas.SimRequest, background\_tasks: star-lette.background.BackgroundTasks, db: sqlalchemy.orm.session.Session) <math>\rightarrow simulation_api.controller.schemas.SimIdResponse
```

Requests simulation to BackgroundTasks.

#### **Parameters**

- sim system (SimSystem) System to be simulated.
- sim\_params (SimRequest) Contains all the information about the simulation request.
- background\_tasks (fastapi.BackgroundTasks) Object needed to request simulation in the background.
- $\bullet \ \ \mbox{\bf db} \ (\mbox{sqlalchemy.orm.Session}) Needed \ for interaction \ with \ \mbox{\bf database}.$

**Returns** sim\_id\_response - Contains information about simulation request, such as simulation ID and others. See SimIdResponse for more information.

**Return type** SimIdResponse

```
simulation_api.controller.tasks._check_chen_lee_params (a: float, b: float, c: float)
Checks that the set of Chen-Lee parameters satisfy chaotic conditions, therefore bound solutions.
```

The conditions are

$$a > 0$$
 and  $b < 0$  and  $c < 0$  and  $a < -(b+c)$ 

**Note:** This conditions are stated in this reference.

## **Parameters**

- **a**  $(float) \omega_x$  parameter.
- **b**  $(float) \omega_u$  parameter.
- **c** (float)  $\omega_{z}$  parameter.

```
simulation api.controller.tasks. create pickle path disk(sim\ id: str) \rightarrow str
```

Creates disk path to simulation results (pickle) by sim id.

simulation\_api.controller.tasks.\_create\_plot\_path\_disk (sim\_id: str, query\_param: Union[simulation\_api.controller.schemas.PlotQueryValues\_HO, simulation api.controller.schemas.PlotQueryValues ChenLee], plot format: str =  $'.png') \rightarrow str$ 

Creates disk path to plots of simulation results by sim\_id.

simulation\_api.controller.tasks.\_pickle (file\_name:  $str, path: str = ", data: Optional[dict] = None) \rightarrow Any$ Saves data to pickle or reads Python object from pickle.

Saves data to pickle if data. Otherwise it will try to read a pickle from path + '/' + file\_name and return the python object stored in it.

## **Parameters**

- **file name** (str) Name of file to be read from or to write on.
- path (str) Path of directory in which the file will be saved or read from.
- data (dict or None, optional) If you want to save data to a pickle, provide the data as dictionary. Default is None.

**Returns** loaded\_object – Object loaded when no data is provided.

**Return type** Any or None

```
simulation api.controller.tasks. plot solution (sim results:
                                                                                     simulation api.controller.schemas.SimResults,
                                                                                                                                                      simula-
                                                                                                                                      system:
                                                                 tion api.controller.schemas.SimSystem, plots basename: str = '00000') \rightarrow List[str]
     Generates relevant simulation's plots and saves them.
```

#### **Parameters**

- sim\_results (SimResults) Simulation results as returned by simulate().
- **system** (SimSystem) System to be simulated.
- plots\_basename (str) Base name of the plots. Actual name of each plot will be <plotbasename>\_<plot\_query\_value>.png, where <plot\_query\_value> is a special tag for each type of plot. In this API, baseplot will always be the value of sim\_id.

**Returns plot\_query\_values** – Names of each type of plot. These are very important since they are needed to access the plots in the API route (these are the possible values for the query param "value" in route /api/results/{sim\_id}/plot).

## **Return type** List[str]

simulation\_api.controller.tasks.\_run\_simulation ( $sim\_params$ : simulation\_api.controller.schemas.SimRequest)  $\rightarrow$  None Runs the requested simulation and stores the outcome in a database.

This function runs the simulation, stores the simulation parameters in a database, stores the simulation result in a pickle and creates and saves relevant plots of the simulation.

Parameters sim\_params (SimRequest) - Contains all the information needed for the simulation.

Returns

Return type None

simulation\_api.controller.tasks.\_sim\_form\_to\_sim\_request (form: Dict[str, str])  $\rightarrow simulation\_api.controller.schemas.SimRequest$  Translates simulation form -from frontend- to simulation request which is understood by backend in \_api\_simulation\_request ().

**Parameters** form (Dict[str, str]) – Simulation request information as obtained by frontend.

**Returns** Simulation request information in a format the backend understands.

Return type SimRequest

```
3.1.1.2.2 simulation_api.model
```

## 3.1.1.2.2.1 Package contents

## 3.1.1.2.2.2 Submodules

## 3.1.1.2.2.3 simulation api.model.crud

This program manages database querys. CRUD comes from: Create, Read, Update, and Delete.

 $simulation\_api.model.crud.\_create\_parameters (\textit{db: sqlalchemy.orm.session.Session, parameters: List[simulation\_api.controller.schemas.ParameterDBSchCreate])} \rightarrow None \\ Insert parameter entry into parameters table.$ 

#### **Parameters**

- **db** (Session) Database Session.
- parameters (List[ParameterDBSchCreate]) Parameter row in parameters' table.

#### Returns

## Return type None

```
simulation\_api.model.crud.\_create\_plot\_query\_values (\textit{db:} sqlalchemy.orm.session.Session, plot\_query\_params: List[simulation\_api.controller.schemas.PlotDBSchCreate]) \rightarrow None
```

# Insert row in plots table (contains plot query params)

#### **Parameters**

- **db** (Session) Database Session.
- plot\_query\_params (List[PlotDBSchCreate]) List of rows to be inserted in plots table.

#### Returns

## Return type None

```
simulation\_api.model.crud.\_create\_simulation (\textit{db: sqlalchemy.orm.session.Session, simulation:} simulation\_api.controller.schemas.SimulationDBSchCreate) \\ \rightarrow \textit{simulation\_api.model.models.SimulationDB} Inserts simulation in simulations table.
```

#### **Parameters**

- **db** (Session) Database Session.
- simulation (SimulationDBSchCreate) Simulation row in simulations table.

Returns db\_simulation - Updated simulation's row.

**Return type** *SimulationDB* 

 $simulation\_api.model.crud.\_{\tt create\_user}(db: sqlalchemy.orm.session, user: simulation\_api.controller.schemas.UserDBSchCreate) \rightarrow simulation\_api.model.models.UserDB \\ Inserts user in users table.$ 

#### **Parameters**

- **db** (Session) Database Session.
- user (UserDBSchCreate) User row in database.

**Returns db\_user** – Updated inserted row (with user\_id.)

Return type UserDB

 $simulation\_api.model.crud.\_get\_all\_simulations (\textit{db: sqlalchemy.orm.session.Session}) \rightarrow Tuple[\textit{simulation\_api.model.models.SimulationDB}] \\ Get all simulation entries in simulations table.$ 

Parameters db (Session) - Database Session.

Returns Querry of all rows in simulations table.

Return type sqlalchemy.orm.Query

 $simulation\_api.model.crud.\_get\_parameters (\textit{db:} sqlalchemy.orm.session.Session, sim\_id: str, param\_type: simulation\_api.controller.schemas.ParamType) \rightarrow Union[List[float], Dict[str, float]]$  Get parameters from parameters table.

#### **Parameters**

- **db** (Session) Database Session.
- $sim_id(str)$  Simulation ID.
- param\_type (ParamType) Type of parameter, wether 'initial condition' or 'parameter'.

 $\textbf{Returns} \ \ \texttt{list} \ \ \textbf{of initial conditions or dict mapping parameter names to parameter values}.$ 

**Return type** List[float] or Dict[str, float]

simulation\_api.model.crud.\_**get\_plot\_query\_values** (db: sqlalchemy.orm.session.Session, sim\_id: str) Return plot query parameters for a given simulation.

## **Parameters**

- **db** (Session) Database Session.
- **sim\_id** (*str*) Simulation ID.

**Returns** Plot query values associated to sim\_id.

**Return type** List[PlotQueryValues]

 $simulation\_api.model.crud.\_get\_simulation$  ( $db: sqlalchemy.orm.session.Session, sim\_id: str$ )  $\rightarrow simulation\_api.model.models.SimulationDB$  Get simulation with specific id from simulation table.

## **Parameters**

- **db** (Session) Database Session.
- **sim\_id** (*str*) Simulation ID.

**Returns** Query with simulation information of sim\_id.

Return type sqlalchemy.orm.Query

simulation\_api.model.crud.\_**get\_username**(db: sqlalchemy.orm.session.Session, user\_id: int)
Gets user from users table.

#### **Parameters**

- **db** (Session) Database Session.
- user id(int)-

**Returns** Query with information about username with given user\_id.

Return type sqlalchemy.orm.Query

## 3.1.1.2.2.4 simulation\_api.model.db\_manager

This module starts the database engine, the database session and the basemodel for the database tables.

## 3.1.1.2.2.5 simulation\_api.model.models

This program creates all the models and tables in the database

```
class simulation_api.model.models.ParameterDB(**kwargs)
```

Bases: sqlalchemy.ext.declarative.api.Base

Parmaeters table model.

Stores parameters and initial conditions of simulations.

```
___init___(**kwargs)
```

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in kwargs.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

## ini\_cndtn\_id

Initial condition position in array of initial conditions.

## param\_id

## param\_key

Name of parameter. Must be one of the required parameters related to the system being simulated.

## param type

Parameter type, wether 'initial condition' or 'parameter'.

#### sim id

Simulation ID.

#### simulation

ORM relationship with simulations' table.

#### value

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Value of 'parameter' or initial contidion.

```
class simulation_api.model.models.PlotDB(**kwargs)
     Bases: sqlalchemy.ext.declarative.api.Base
     Plots table model.
     Stores query parameter values of plots needed to access simulation results via GET in route /api/results/{sim_id}/plot?value={plot_query_value}.
     ___init___(**kwargs)
          A simple constructor that allows initialization from kwargs.
          Sets attributes on the constructed instance using the names and values in kwargs.
          Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.
     plot_id
          Primary key.
     plot_query_value
          Label of each plot, used as query value for query param value in route /api/results/{sim_id}/plot.
     sim id
          Simulation ID.
     simulation
          ORM relationship with simulations' table.
class simulation api.model.models.SimulationDB(**kwargs)
     Bases: sqlalchemy.ext.declarative.api.Base
     Simulation Status table model.
      init (**kwargs)
          A simple constructor that allows initialization from kwargs.
          Sets attributes on the constructed instance using the names and values in kwargs.
          Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.
     date
     message
          Message with further information about the simulation status.
     method
          Integration method.
```

```
parameters
          ORM relationship with parameters' table.
     plots
          ORM relationship with plots' table.
     route_pickle
          API route to GET simulation results in pickle format.
     route plots
          API route to GET simulation plots.
     route results
          API route to GET simulation results displayed in frontend web page.
     sim_id
          Simulation ID.
     success
          Tells if the simulation was successful or not.
     system
          Simulated system.
     user
          ORM relationship with users' table.
     user_id
          user_id.
              Type Foreign key
class simulation api.model.models.UserDB(**kwargs)
     Bases: sqlalchemy.ext.declarative.api.Base
     Users table model.
     This table stores basic user information.
     Note: hash_value and this users table is not appropriately used yet because logging is not yet implemented in the app.
```

\_\_\_init\_\_\_(\*\*kwargs)

A simple constructor that allows initialization from kwargs.

```
Sets attributes on the constructed instance using the names and values in kwargs.
```

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

## hash value

Hash value of the usser's password.

#### simulations

ORM relationship with simulations' table.

user id

username

## 3.1.1.2.3 simulation\_api.simulation

## 3.1.1.2.3.1 Package contents

## 3.1.1.2.3.2 Submodules

## 3.1.1.2.3.3 simulation api.simulation.demo run simulation

Test for simulations defined in simulation module

## 3.1.1.2.3.4 simulation\_api.simulation.simulations

This module simulates mechanical systems

```
 \textbf{class} \  \, \text{simulation\_api.simulations.ChenLeeAttractor} \, (\textit{t\_span: Optional[Tuple[float, float]]} = [0, \, 400], \, \textit{t\_eval: Optional[tuple]} = \\ None, \, ini\_cndtn: \, \textit{List[float]} = [10.0, \, 10.0, \, 0.0], \, \textit{params: dict} = \{'a': \, 3.0, \, 'b': \\ -5.0, \, 'c': -1.0\}, \, \textit{method: str} = 'RK45', \, \textit{user\_name: Optional[str]} = None)
```

 $Bases: \verb|simulation_api.simulation.simulations.Simulation|\\$ 

Simulates Chen-Lee Attractor.

а

 $\omega_x$  parameter.

Type float

b  $\omega_y$  parameter. Type float c  $\omega_z$  parameter. Type float

## **Notes**

The Chen-Lee Attractor is a dynamical system defined by:<sup>1</sup>

$$\frac{d\omega_x}{dt} = -\omega_y \omega_z + a \,\omega_x$$

$$\frac{d\omega_y}{dt} = \omega_z \omega_x + b \,\omega_y$$

$$\frac{d\omega_z}{dt} = \frac{1}{3} \omega_x \omega_y + c \,\omega_z$$

Its origin is closely related to the motion of a rigid body in a rotating frame of reference.

## References

```
\_init\_(t\_span: Optional[Tuple[float, float]] = [0, 400], t\_eval: Optional[tuple] = None, ini\_cndtn: List[float] = [10.0, 10.0, 0.0], params: dict = {'a': 3.0, 'b': -5.0, 'c': -1.0}, method: str = 'RK45', user\_name: Optional[str] = None) \rightarrow None Extends Simulation.\_\_init\_\_()
```

Adds attributes ChenLeeAttractor.a, ChenLeeAttractor.b and ChenLeeAttractor.c.

## **Parameters**

•  $ini\_cndtn(array\_like, shape (3,))$  – Initial condition of 1D Harmonic Oscillator. Convention:

```
"a": float, # `\omega_x` parameter.
"b": float, # `\omega_x` parameter.
```

(continues on next page)

<sup>&</sup>lt;sup>1</sup> https://doi.org/10.1142/S0218127403006509

```
(continued from previous page)
```

```
"c": float,
                                             # `\omega_z` parameter.
                  Default is { "a": 3.0, "b": -5.0, "c": -1.0}.
dyn_sys_eqns(t: float, w: List[float]) \rightarrow List[float]
     Chen-Lee Dynamical system definition
     Note: Overwrites Simulation.dyn sys egns.
         Parameters
             • w (array_like, shape (3,)) - Vector of angular velocity. Convention: w = [\omega_x, \omega_y, \omega_z].
             • t (float) - Time.
         Returns dwdt – Dynamical system equations of Chen Lee attractor evaluated at w.
         Return type array_like, shape (3,)
system = 'Chen-Lee-Attractor'
class simulation_api.simulation.simulations.HarmonicOsc1D(t_span: Optional[Tuple[float, float]] = [0, 6.283185307179586], t_eval: Op-
                                                                             tional[tuple] = None, ini\_cndtn: List[float] = [0.0, 1.0], params: dict = {'k': 1.0, tional[tuple]}
                                                                              'm': 1.0}, method: str = 'RK45', user_name: Optional[str] = None)
     Bases: simulation_api.simulation.simulations.Simulation
     1-D Harmonic Oscillator simulation
     m
          Mass of object.
               Type float
```

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k

Force constant of harmonic oscilltor.

Type float

#### **Notes**

The hamiltonian describing the Harmonic Oscillator is defined dy

$$H = \frac{1}{2m}p^2 + \frac{1}{2}kq^2$$

```
\_init\_(t\_span: Optional[Tuple[float, float]] = [0, 6.283185307179586], t\_eval: Optional[tuple] = None, ini\_cndtn: List[float] = [0.0, 1.0], params: dict = {'k': 1.0, 'm': 1.0}, method: str = 'RK45', user\_name: Optional[str] = None) \rightarrow None Extends Simulation.\_\_init\_\_()
```

Adds attributes HarmonicOsc1D.m and HarmonicOsc1D.k.

## **Parameters**

• ini\_cndtn (array\_like, shape (2,)) - Initial condition of 1D Harmonic Oscillator. Convention:

```
"m": float,  # Mass of object.
   "k": float,  # Force constant of harmonic oscilltor.
}
```

```
Default is {"m": 1., "k": 1.}.
```

**dyn\_sys\_eqns** (*t: float*, *y: List[float]*) → List[float] Hamilton's equations for 1D-Harmonic Oscillator.

Trainition's equations for 1D-Trainionic Oscillator.

Note: Overwrites Simulation.dyn sys egns.

#### **Parameters**

- t (float) Time of evaluation of Hamilton's equations.
- $\mathbf{y}$  (array\_like, shape (2,)) Canonical coordinates. Convention:  $\mathbf{y} = [q, p]$  where q is the generalised position and p is the generalised momentum.

**Returns dydt** – Hamilton's equations for 1D Harmonic Oscillator. dydt =  $\left[\frac{dq}{dt}, \frac{dp}{dt}\right] = \left[\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial q}\right]$ 

```
Return type array_like, shape (2,)
system = 'Harmonic-Oscillator'
class simulation_api.simulation.simulations.Simulation (t_span: Optional[List[float]] = None, t_eval: Optional[list] = None, ini_cndtn: Op-
                                                                           tional[list] = None, params: Optional[dict] = None, method: Optional[str] = 'RK45',
                                                                           user_name: Optional[str] = None)
     Bases: object
     Simulation of a continuous dynamical system described by first order coupled differential equations.
     t_span
          Interval of integration (t0, tf).
               Type List[float, float] or None
     t eval
          Times at which to store the computed solution, must be sorted and lie within t_span.
               Type array_like or None
     ini_cndtn
          Initial condition of simulation, its specification depends on the system being simulated.
               Type array_like or None
     params
          Contains all the parameters of the simulation (e.g. for the harmonic oscillator self.params = {"m": 1., "k": 1.})
               Type dict or None
     method
          Method of integration.
               Type str, optional
     user_name
           Username that instantiated the simulation.
               Type str or None
     date
          UTC date and time of instantiation of object.
               Type datetime (str)
```

#### results

Results of simulation.

```
Type scipy.integrate._ivp.ivp.OdeResult or None
```

 $\_$ \_init $\_$ (t\_span: Optional[List[float]] = None, t\_eval: Optional[list] = None, ini\_cndtn: Optional[list] = None, params: Optional[dict] = None, method: Optional[str] = 'RK45', user\_name: Optional[str] = None)  $\rightarrow$  None Initializes all self attributes except self.system

```
dyn_sys_eqns(t: float, y: List[float]) \rightarrow List[float]
```

Trivial 2D dynamical system. Just for reference.

**Note:** The actual simulations that inherit this class will replace this method with the relevant dynamical equations.

## $simulate() \rightarrow scipy.integrate\_ivp.ivp.OdeResult$

Simulates self.system abstracted in self.dyn\_sys\_eqns and using scipy.integrate.solve\_ivp.

## Returns

#### self.results -

Bunch object with the following fields defined:

- t [ndarray, shape (n\_points,)] Time points.
- y [ndarray, shape (n, n\_points)] Values of the solution at t.
- sol [OdeSolution or None] Found solution as OdeSolution instance; None if dense\_output was set to False.
- **t\_events** [list of ndarray or None] Contains for each event type a list of arrays at which an event of that type event was detected. None if events was None.
- **y\_events** [list of ndarray or None] For each value of t\_events, the corresponding value of the solution. None if events was None.
- nfev [int] Number of evaluations of the right-hand side.
- njev [int] Number of evaluations of the Jacobian.
- **nlu** [int] Number of LU decompositions.
- **status** [int] Reason for algorithm termination: -1, Integration step failed; 0, The solver successfully reached the end of tspan; 1, A termination event occurred.
- message [string] Human-readable description of the termination reason.

success [bool] True if the solver reached the interval end or a termination event occurred (status >= 0).

Return type OdeResult

system = None

Name of system.

simulation\_api.simulation.simulations.Simulations = {'Chen-Lee-Attractor': <class 'simulation\_api.simulation.simulations.ChenLee

Maps the names of the available systems to their corresponding classes.

Warning: Must be updated each time a new simulation is added (add the new relevant item to the dictionary).

## 3.1.1.3 Submodules

## 3.1.1.3.1 simulation API.config module

General configurations of our API.

## 3.1.2 Add a new simulation

Keep in mind that the systems we can add to our API are those that can be integrated by scipy.integrate.solve\_ivp. Those are basically first order coupled differential equations i.e. systems of the form

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}, t).$$

If you want to add a new simulation to this API just follow the steps described below.

## 3.1.2.1 1. Add the simulation to simulations module

- 1. Add a relevant class to <code>simulations</code>. This class will define the relevant parameters used in the simulation as well as its dynamic equations. It must inherit <code>Simulation</code> and must have the same structure as <code>HarmonicOsclD</code> and <code>ChenLeeAttractor</code>. Don't forget to test your simulation by playing around in <code>demo\_run\_simulation</code>.
- 2. Don't forget to add the attribute system to your class. The value of this attribute must be the name of the system separated by dashes. Use only alphanumerical characters and dashes.

3. Add the relevant simulation class you just created to the dict Simulations. This will tell the API that the simulation exists and it is available.

## 3.1.2.2 2. Add relevant schemas and models to schemas

Follow the steps mentioned below –some of them may not make sense at first glance, but until you write the code.

- 1. Add the system attribute value of the recently created class to SimSystem.
- 2. Create a class that inherits SimForm. It must be similar to HOSimForm and ChenLeeSimForm. This class will be used to check the simulation information provided in frontend.
- 3. Add a relevant item -related to the class created in the last numeral- to the dict SimFormDict. This will map the name of the system to its simulation form model.
- 4. Add a new class similar to HOParams and ChenLeeParams. The names of the attributes must match the names of the parameters defined in the relevant simulation class, created in the first numeral of this list.
- 5. Add an appropriate item to the dict SimSystem\_to\_SimParams.
- 6. Create an appropiate dict similar to params\_mapping\_HO and params\_mapping\_ChenLee.
- 7. Add an appropriate item to the dict system\_to\_params\_dict.
- 8. Create a new class similar to PlotQueryValues\_HO and PlotQueryValues\_ChenLee.
- 9. Add an appropiate item to PlotQueryValues.

If you do not understand some of the steps above or how to implement them, refer to *the documentaton* of the relevant classes or schemas for the already available systems –Chen-Lee Attractor or Harmonic Oscillator–, it may enlighten you.

## 3.1.2.3 3. Add relevant plots to \_plot\_solution()

Here you can add two or three intersting plots related to the simulation you just added and tested. The code that generates the plots must be placed in simulation\_api.controller.tasks.\_plot\_solution().

A few things to take into account:

- 1. We use matplotlib, but we use the class Figure directly, we do not use pyplot. This is related to some problems that may arise with the pyplot package and the web applocation backend, as mentioned in matplotlib's documentation.
- 2. Note that the plots related to the simulations are defined in an if or elif block each one. Add a new block for the simulation you want to add.
- 3. The first two lines of code that generate each plot related to the recently created simulation must look something like:

```
plot_query_value = PlotQueryValues_HO.phase.value
plot_query_values.append(plot_query_value)
```

For each generated plot,we define a plot\_query\_value that comes directly from the class defined in item number 8 of the *last section*. In the example given above, the class was named PlotQueryValues\_HO, the attribute related to the plot\_query\_value of the relevant plot was named coord and the value of the latter is accessed by using .value. Each plot\_query\_value is appended to the list plot\_query\_values, which is the return value of \_plot\_solution(). This item is very important, since the values we define here are used to name the plots as well as to look them up.

4. Finally, the last line of code that generates each plot must be:

```
fig.savefig(_create_plot_path_disk(plots_basename, plot_query_value))
```

This will ensure that the name of the plot has always the same format

## 3.1.2.4 4. Add relevant form entries in frontend

Modify appropriately the template simulation\_api/templates/request-simulation.html. This template is the one that asks for the simulation parameters in the frontend.

Some things to take into account:

- 1. Note that each system has its own if or elif block. Stick to this convention and add a new block related to the new simulation (the new system).
- 2. In the if block mentioned above there are only two main things the form should ask for: initial conditions and parameters of simulation.
- 3. For the initial conditions the value of the HTML attribute name should start with the string "ini" followed by the index in the initial condition array defined in your simulation class attribute ini\_cndtn. For example, for the harmonic oscillator the convention of initial condition is

## 3.1.2.5 5. Modify results.html template to show results

Finally, we need to add a relevant elif block to the template simulation\_api/templates/results.html. This template should show the generated plots, give the option to download them with a button and give the option to download the pickle file as well.

**simulation\_api** Initialization of web application.

simulation\_api.controller The core package of our API. Here you can find the main app, schemas and background tasks.

simulation\_api.model Database-related package.

**simulation\_api.simulation** Simulation-related package. Here you can find all the programs we use to simulate the available systems.

**simulation\_api.config** Configuration module. Some very basic configurations of our web application.

## **CHAPTER**

# **FOUR**

# **INDICES AND TABLES**

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# A SPECIAL AKNOWLEDGEMENT

To Camilo Hincapié who guided me in this process.

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