PHYS Simulation API

Release 0.0.1

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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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2 GETTING STARTED

CHAPTER

ONE

HISTORY

PHYS Simulation API started as a way of learning to develop a web application. 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.

4 Chapter 1. History

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 /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	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	Harmonic-Oscillator, Chen-Lee-Attractor		
IntegrationMethods	IntegrationMethods				
	List of available integration methods.				
	For more information see scipy.integrate.solve_ivp.				
	type	string	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			
	type	integer		
• username	Username			
	type	string		
• sim_sys	SimSystem			
	type	string		
• sim_status_path	Sim Status Path			
	type	string		
sim_pickle_path	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

Schema of the Simulation	Satus.				
ype	object				
properties					
• 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	number		
 method 	IntegrationMethods				
	type	string			
route_pickle	Route Pickle				
	type	string			
route_results	Route Results				
	type	string			
route_plots	Route Plots				
	type	string			
plot_query_values	PlotQueryValues				
	type	array			
	items	anyOf	PlotQueryValues_HO		
			type	object	
			additionalProperties	type	string
			PlotQueryValues_0		
			type	object	continues on poyt page

continues on next page

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				
• message	Message					
	type	string				
definitions						
SimSystem	SimSystem					
	List of available systems for	or simulation.				
	type	string				
	enum Harmonic-Oscillator, Chen-Lee-Attractor					
 IntegrationMethods 	IntegrationMethods					
	List of available integration methods.					
	For more information see scipy.integrate.solve_ivp.					
	type	string				
	enum	RK45, RK23				
•	PlotQueryValues_HO					
PlotQueryValues_HC		nt plot generated automatically				
		Oscillator simulation is reque	sted.			
	type	string				
	enum coord, phase					
•	1 tot Query values_Cherizee					
PlotQueryValues_Ch	ues_CherlList of tags of each different 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!

2.2.1 1. Request Simulation

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

```
>>> import requests
>>> import os
>>> from time import sleep
>>>
>>>
>>> # Prepare the simulation request
>>> sim_system = "Chen-Lee-Attractor"
>>> sim_request = {
      "system": sim_system,
>>>
      "username": "PHYSSimulation",
>>>
      "t_span": [0, 200],
>>>
      "t_steps": 1e5,
>>>
```

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```
"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(" }")
Simulation Request Response
```

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```
HTML status code: 200

Response:

{
    'sim_id': e5f6d0e0719b45fea4aa9f098e12e7c3,
    'user_id': 1,
    'username': PHYSSimulation,
    'sim_sys': Chen-Lee-Attractor,
    'sim_status_path': /api/simulate/status/e5f6d0e0719b45fea4aa9f098e12e7c3,
    'sim_pickle_path': /api/results/e5f6d0e0719b45fea4aa9f098e12e7c3/pickle,
    'message': (When -and if- available) request via GET your simulation'sstatus in route 'sim_status_path' or download your_
    →results(pickle fomat) via GET in route 'sim_pickle_path',
}
```

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}.

```
>>> # Wait until the simulation is done
>>> sleep(5)
>>>
>>> # Get simulation ID
>>> sim_id = sim_request_response.json()["sim_id"]
>>>
>>> # Simulation status route
>>> sim_status_route = f"/api/simulate/status/{sim_id}"
>>>
>>> # Request simulation status via HTTP using `requests` module
>>> sim_status_response = requests.get(url + sim_status_route)
>>>
>>> # Print response
>>> print(
>>>
      "Simulation status Response",
      "_____",
>>>
      f"HTML status code: {sim_status_response.status_code}",
>>>
```

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(continued from previous page)

```
>>>
       "Response:",
       " { ",
>>>
       sep=' \n',
>>>
>>> )
>>> for key, v in sim_status_response.json().items():
       print(f"
                      '{key}': {v},")
>>> 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.

2.2. Examples

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

```
>>> # 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)
```

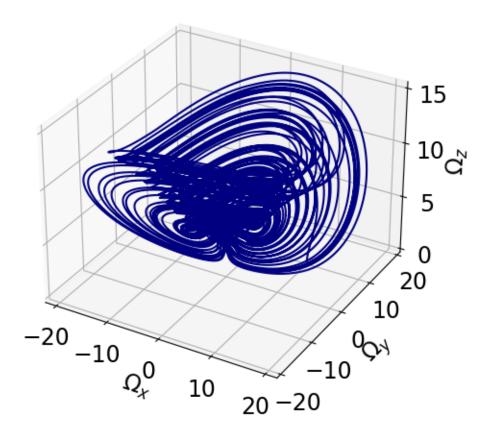
The generated file is named simulation.pickle and contains all the information of the simulation results.

Finally, lets download the plots

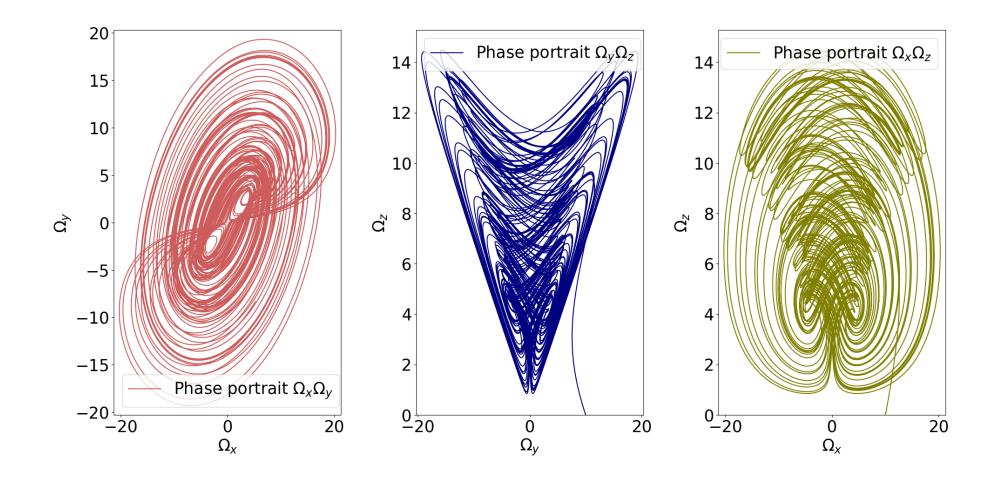
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```
>>> # Plots download route
>>> plots_route = sim_status_response.json()["route_plots"]
>>>
>>> # Plot query values
>>> plot_query_values = sim_status_response.json()["plot_query_values"]
>>>
>>> for qv in plot_query_values:
        # Construct 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)
>>>
        # 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

```
async simulation_API.controller.main.api_results_sim_id_pickle(sim_id: str)
Download pickle of previously requested simulation.
```

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

Returns FileResponse containing the simulation results in pickle format.

Return type starlette.responses.FileResponse

async simulation_API.controller.main.api_results_sim_id_plot (sim_id: str, value: Union[simulation_API.controller.schemas.PlotQueryValues_HO, simulation_API.controller.schemas.PlotQueryValues_ChenLee])

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: $sqlalchemy.orm.session.Session = Depends(get_db)) \rightarrow simulation_API.controller.schemas.SimIdResponse$

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(get_db)) → simulation API.controller.schemas.SimStatus Obtains status of requested simulation.

Parameters

- sim id(str) ID of the simulation.
- 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:
                                                                                                                                      star-
                                                                                  lette.exceptions.HTTPException)
```

Handles 404 exceptions by rendering a template.

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

Starts and ends session in each route that needs database access

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

3.1. The Code 21 **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.

Return type 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 =
                                                                                Form(Ellipsis), t steps: int = Form(Ellipsis), method:
                                                                                                                                           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.

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- 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.

async simulation_API.controller.main.simulate_status_sim_id(request: starlette.requests.Request, sim_id: str, db:

sqlalchemy.orm.session.Session = Depends(get_db))

Shows simulation status for a given simulation via its sim id.

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.

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 simulation_API.controller.schemas.HOParams.

a: float

 ω_x parameter.

b: float

 ω_{y} parameter.

c: float

 ω_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.

3.1. The Code

ini0: Optional[float]

 ω_x initial condition.

ini1: Optional[float]

 ω_n initial condition.

ini2: Optional[float]

 ω_z initial condition.

param0: Optional[float]

Parameter of name a.

param1: Optional[float]

Parameter of name b.

param2: Optional[float]

Parameter of name 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 simulation_API.controller.schemas.ChenLeeParams.

k: float

Force constant of object.

m: float

Mass of object.

```
class simulation_API.controller.schemas.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 m.

param1: Optional[float]
    Parameter of name k.

sim_sys: simulation_API.controller.schemas.SimSystem
    System to be simulated.

class simulation_API.controller.schemas.IntegrationMethods(value)
    Bases: str, enum.Enum
```

Note: For more information about these integration methods see scipy.integrate.solve_ivp.

List of available integration methods

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.
         orm model = True
```

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```
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.
```

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,
                                                                 float = 0.3141592653589793, t steps:
                                                                                                           int = 0, method:
                                                          tion API.controller.schemas.IntegrationMethods = 'RK45')
     Bases: pydantic.main.BaseModel
    Basemodel of schema used to Request a Simulation in Frontend.
      Warning: Needs update each time a new simulation is added:
        1. Create a new appropriate class similar to <code>HOSimForm</code> or to <code>ChenLeeSimForm</code>.
        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.

Schema needed to request simulations via POST in /api/request/{sim_system}.

```
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
```

For the attributes that do not have a description see <code>simulation_API.simulation.simulations.Simulation</code>.

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.
     system: 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
class simulation API.controller.schemas.SimStatus(*, sim id:
                                                                          str, user id:
                                                                                          int, date:
                                                                                                       datetime.datetime, system:
                                                            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,
                                                             plot_query_values: List[Union[simulation_API.controller.schemas.PlotQueryValues_HO,
                                                             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]

 $\verb|plot_query_values: Optional[List[Union[simulation_API.controller.schemas.PlotQueryValues_HO, simulation_API.controller.schemas.PlotQueryValues_HO, simul$

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, 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.Chem
Maps the name of each available system to its parameters model

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, method: str = None, $route_pickle$: str = None, route

Bases: simulation API.controller.schemas.SimulationDBSchBase

Model for API type checking when reading a row in simulations 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
    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': 'c

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

```
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) \rightarrow simulation_API.controller.schemas.SimIdResponse
```

Requests simulation to BackgroundTasks.

Parameters

• sim system (SimSystem) - System to be simulated.

schema given by simulation_API.controller.schemas.SimRequest.)

- 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

$$a+b+c<0$$
 and $ab+bc+ca>0$ and $abc>0$

and due to symmetry of Chen-Lee system, cyclic permutations of a, b and c.

Note: This conditions are stated in this reference.

Parameters

- **a** $(float) \omega_x$ parameter.
- **b** $(float) \omega_u$ parameter.
- c (float) ω_z parameter.

```
\verb|simulation_API.controller.tasks._{\verb|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, system: simulation_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 (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\_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._create_user(db: sqlalchemy.orm.session.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*

 $simulation_API.model.crud._get_all_simulations$ (db: sqlalchemy.orm.session.Session) \rightarrow Tuple[$simulation_API.model.models.SimulationDB$] 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.
- $\bullet \ param_type \ (\texttt{ParamType}) Type \ of \ parameter, \ we ther \ \texttt{'initial condition'} \ or \ \texttt{'parameter'}.$

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

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 simulations 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.

 $\textbf{Return type} \ \texttt{sqlalchemy.orm.Query}$

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 kwarqs.
```

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

```
class simulation_API.simulations.ChenLeeAttractor (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: <math>str = 'RK45', user_name: Optional[str] = None)
```

Bases: simulation_API.simulation.simulations.Simulation

Simulates Chen-Lee Attractor.

а

 ω_x parameter.

Type float

b ω_y parameter. Type float c ω_z parameter. Type float

Notes

The Chen-Lee Attractor is a dynamical system defined by:¹

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

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

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

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\_API.simulation.simulations.Simulation.__init<math>\___()
```

Adds attributes a, b and 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)

¹ 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 API. simulation. simulations. 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
     k
          Force constant of harmonic oscilltor.
```

3.1. The Code 49

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 $simulation_API.simulation.simulations.Simulation.__init___()$

Adds attributes m and 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.}.

 $\texttt{dyn_sys_eqns} \; (\textit{t: float}, \textit{y: List[float]}) \; \rightarrow \text{List[float]}$

Hamilton's equations for 1D-Harmonic Oscillator.

Note: Overwrites simulation_API.simulation.simulations.Simulation.dyn_sys_eqns.

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 simulations. This class will define the relevant parameters used in the simulation as well as its dynamic equations. It must inherit Simulation and must have the same structure as HarmonicOsclD and ChenLeeAttractor. Don't forget to test your simulation by playing around in demo_run_simulation.
- 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 appropriate dict similar to params_mapping_HO and params_mapping_ChenLee.
- 7. Add an appropiate item to the dict system_to_params_dict.
- 8. Create a new class similar to PlotQueryValues_HO and PlotQueryValues_ChenLee.
- 9. Add an appropriate 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_endtn. 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

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A SPECIAL AKNOWLEDGEMENT

To Camilo Hincapié who guided me in this process.

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