Thematic services

Computational physics

National Initiatives for Open Science in Europe – H2020 Research and Innovation action – contract no. 857645

Schrödinger Web Service

RESTful web service for solving multidimensional time-independent Schrödinger equation using Hermite DVR approach

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Service Description - Schrödinger API

- **RESTful web service for solving multidimensional time-independent Schrödinger equation using Hermite DVR approach**
  - solution of **one-dimensional**, **two-dimensional** and **three-dimensional** time-independent Schrödinger equation based on the Gauss-Hermite Discrete Variable Representation (DVR) approach
  - The **Schrödinger** API is available at: https://schrodinger.chem-api.finki.ukim.mk/

Service Description - Schrödinger API

The solution of **1D** Schrödinger equation is illustrated in the case of following model potentials:

- Morse potential
- Simple Harmonic Oscillator (SHO) potential
- Sombrero potential (Mexican hat)
- Woods-Saxon potential

Solutions of **2D** and **3D** Schrödinger equations are illustrated for the following two model potentials:

- 2D Morse potential
- 2D SHO potential
- 3D Morse potential

1D Morse potential

Returns one-dimensional Morse potential V(x):

$$V(x) = D * (1 - exp(-a * (x - x0)))^2 - D$$

Parameters:

npts - number of points (default value 10)
D - dissociation depth (default value 3.0)
a - inverse "width" of the potential (default value 0.5)
x0 - equilibrium bond distance (default value 0.0)
prec - precision (default value 6)

1D SHO potential

Returns one-dimensional harmonic oscillator potential *V(x)* with wavenumber *k*:

$$V(x) = 1/2 * k * (x - x0)^2$$

Parameters:

npts - number of points (default value 5)

k - wavenumber of the SHO potential (default value 1.0)

x0 - displacement from origin (default value 0.0)

prec - precision (default value 8)

1D Sombrero potential

Returns one-dimensional version of the sombrero potential and requires $a < 0$ and $b > 0$:

$$V(x) = a * x^2 + b * x^4$$

Request URL

```
https://schrodinger.chem-api.finki.ukim.mk/1dHermiteSombrero?npts=5&a=-5&b=1&prec=8
```

Server response

Code	Details
200	Response body

```
[-3.31729755 -3.29056942 -1.70943058 -1.67240256  2.48970011]
```

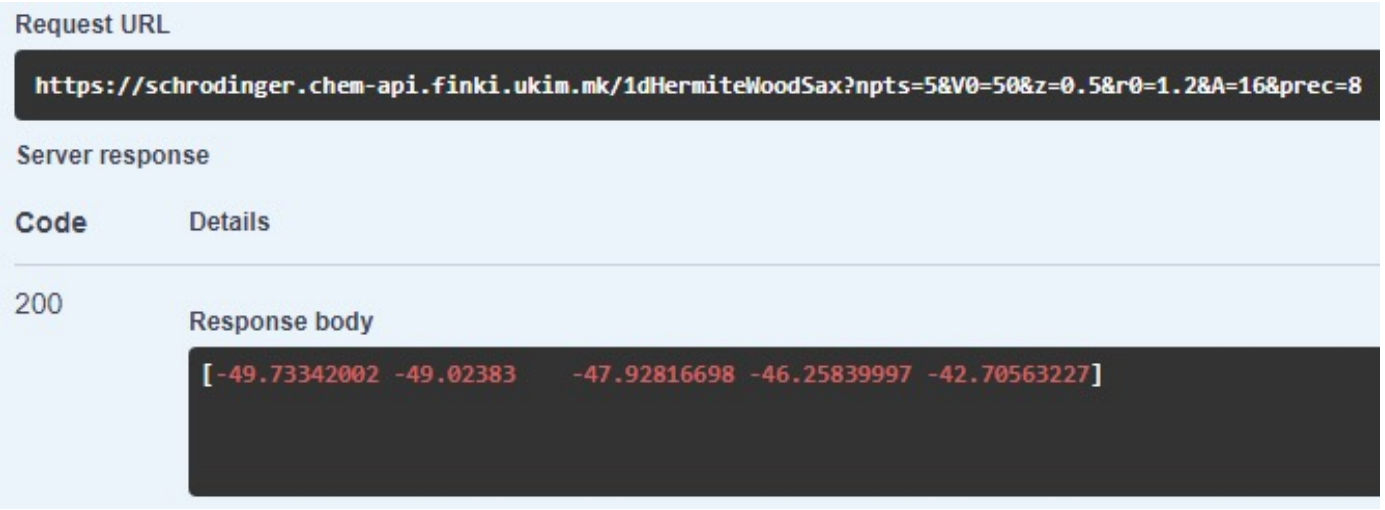
Parameters:

npts - number of points (default value 10)
D - dissociation depth(default value 3.0)
a - inverse "width" of the potential (default value 0.5)
x0 - equilibrium bond distance (default value 0.0)
prec - precision (default value 6)

1D Woods-Saxon potential

Returns a Woods-Saxon potential

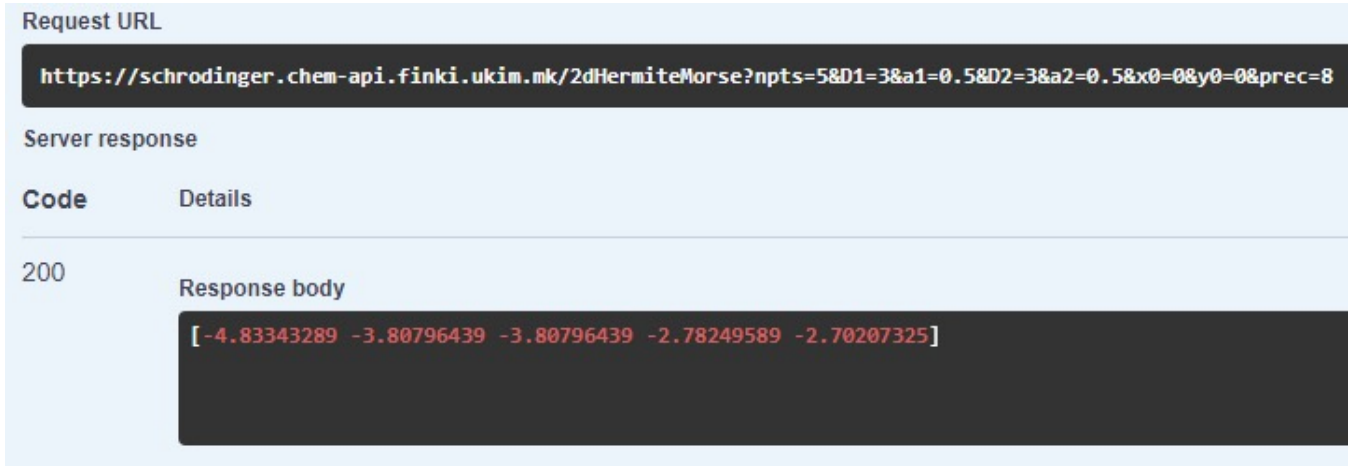
$V(r) = - V0 / (1. + exp((r - R) / z))$ where $R = r0 * A^{(1/3)}$



Parameters:

npts - number of points (default value 5)
V0 - potential depth (default value 50.0)
z - surface thickness (default value 0.5)
r0 - rms nuclear radius (default value 1.2)
A - mass number (default value 16)
prec - precision (default value 8)

2D Morse potential



Parameters:

npts - number of points (default value 5)

D1 - dissociation depth for x (default value 3.0)

a1 - inverse "width" of the potential for x (default value 0.5)

x0 - equilibrium bond distance for x (default value 0.0)

D2 - dissociation depth for y (default value 3.0)

a2 - inverse "width" of the potential for y (default value 0.5)

y0 - equilibrium bond distance for y (default value 0.0)

prec - precision (default value 6)

2D SHO potential

Request URL

```
https://schrodinger.chem-api.finki.ukim.mk/2dHermiteSho?npts=5&k=1&x0=0&y0=0&prec=8
```

Server response

Code	Details
200	Response body

```
[1. 2. 2. 3. 3.]
```

Parameters:

npts - number of points (default value 5)

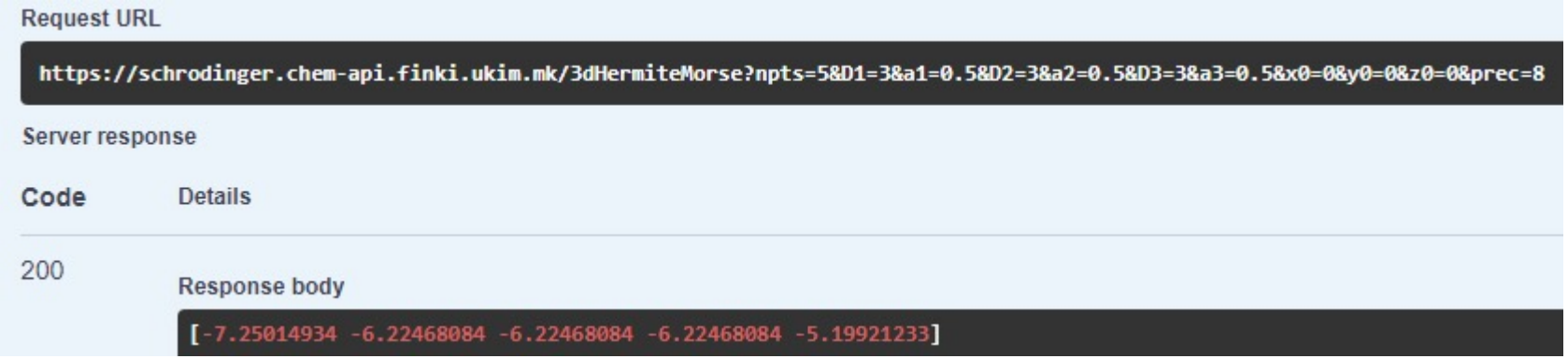
k - wavenumber of the SHO potential (default value 1.0)

x0 - x displacement from origin (default value 0.0)

y0 - y displacement from origin (default value 0.0)

prec - precision (default value 8)

3D Morse potential



Parameters:

npts - number of points (default value 5)

D1 - dissociation depth for x (default value 3.0), D2 - dissociation depth for y (default value 3.0), D3 - dissociation depth for z (default value 3.0)

a1 - inverse "width" of the potential for x(default value 0.5), a2 - inverse "width" of the potential for y(default value 0.5), a3 - inverse "width" of the potential for z(default value 0.5)

x0 - equilibrium bond distance for x (default value 0.0), y0 - equilibrium bond distance for y (default value 0.0), z0 - equilibrium bond distance for z (default value 0.0)

prec - precision (default value 6)

Service DEMO

Jupyter notebook link:

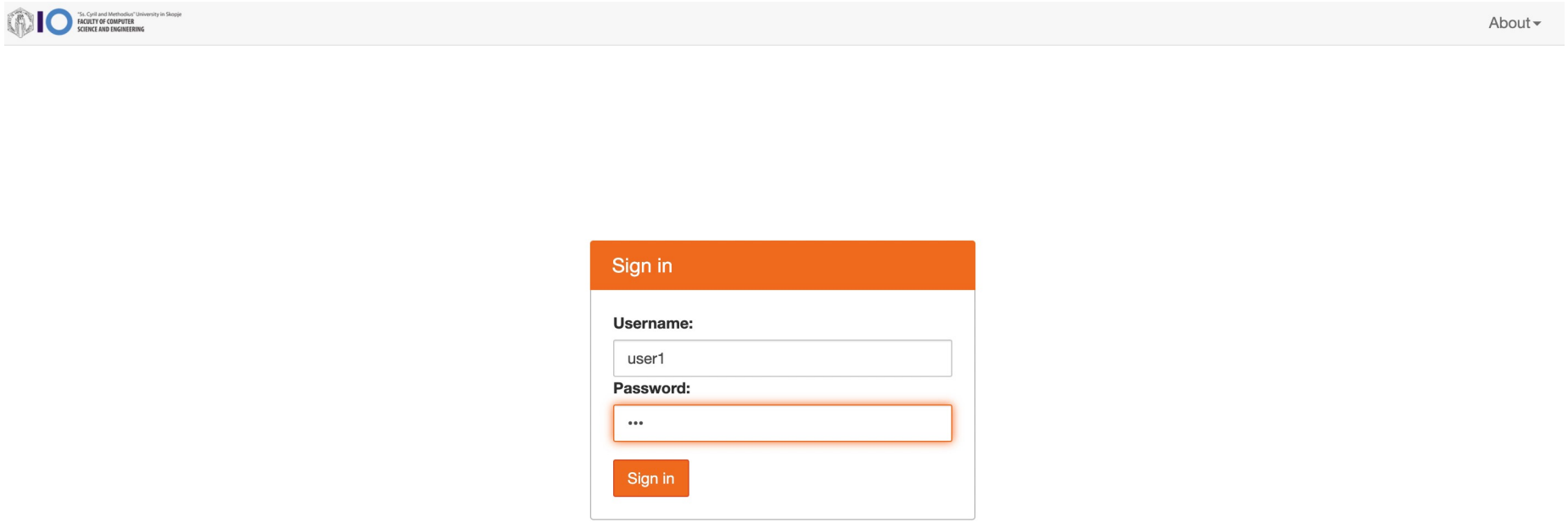
https://notebooks.finki.ukim.mk/user/user1/notebooks/SchrodingerAPI.ipynb

User: user1

Password: User1DEMO

The service demo video can be seen on the next slide

Service DEMO video



Gaussian Web Service

RESTful web service for fitting repulsive potentials in density-functional tight-binding with Gaussian process regression

National Initiatives for Open Science in Europe – H2020 Research and Innovation action – contract no. 857645

Service Description - Gaussian API

- **RESTful web service for fitting repulsive potentials in density-functional tight-binding with Gaussian process regression**
  - The Gaussian API is available at: https://gaussian.chem-api.finki.ukim.mk/ .

Service Description - Gaussian API

- It provides two methods:
  - GPrep (POST method) and
  - GPrepRemote (GET method).

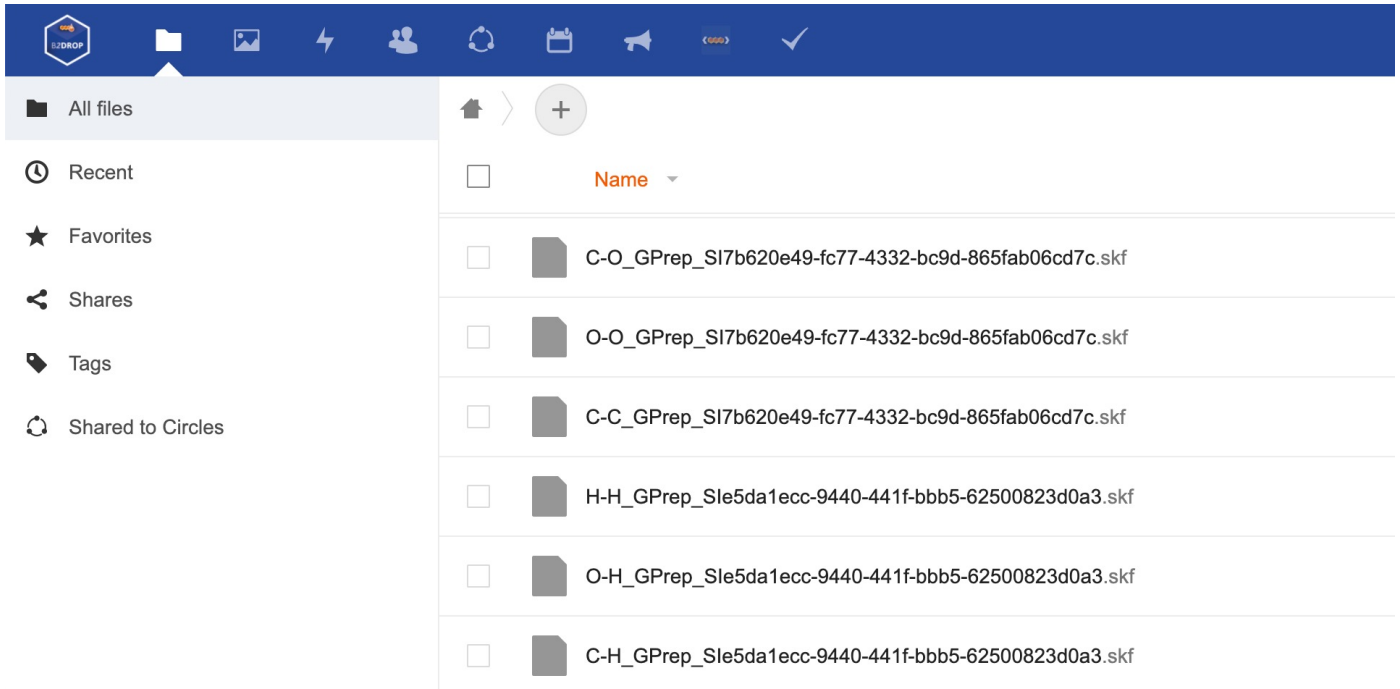
- In case of **GPrep**, the user should provide an input file by browsing the file system on the local device, while in case of **GPrepRemote** the user should provide a public URL where the input file can be accessed.

  - The provided URL should be a direct link to a public file (https://gaussian.chem-api.finki.ukim.mk/static/reference_data.xyz) or public **Dropbox** link (https://www.dropbox.com/s/qnk7r3ey6pkfzb9/reference_dataB.xyz?dl=0) or public **B2DROP** link (https://b2drop.eudat.eu/s/QWPRFGwYHEno99P).

B2DROP

- Secure and trusted data exchange service for researchers and scientists to keep their research data synchronized and up-to-date and to exchange with other researchers.
- The output Slater-Koster files (.skf) with potentials will be uploaded to the user **B2DROP** account

  https://b2drop.eudat.eu/apps/files/
- The user should log in to **B2DROP** (preferably by using her/his institutional account) and to generate username and password.

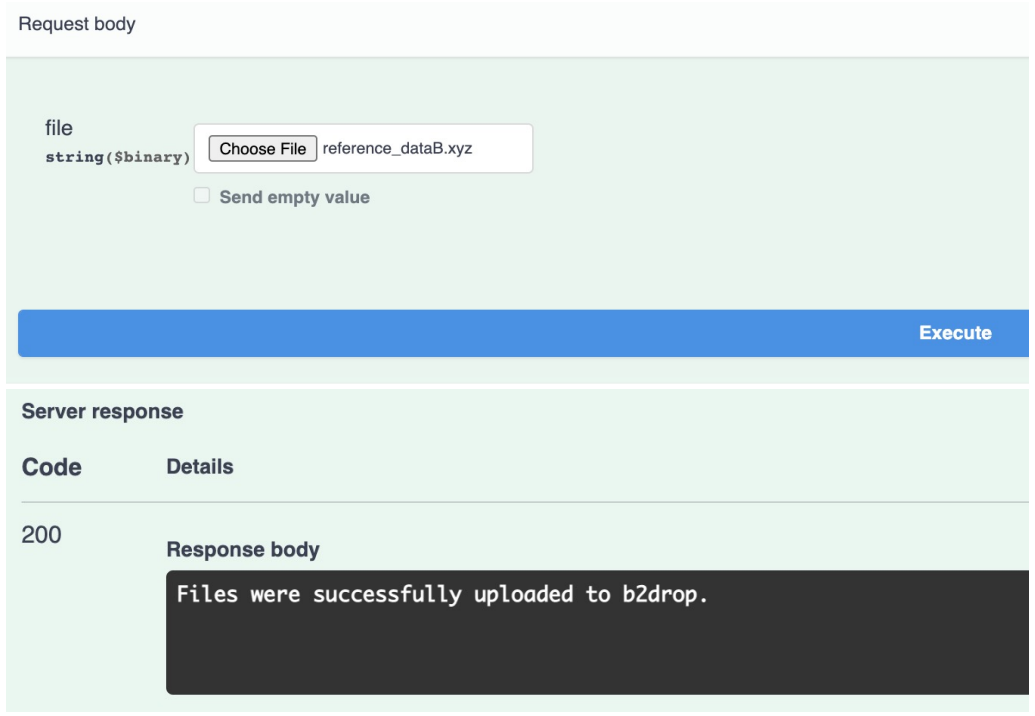


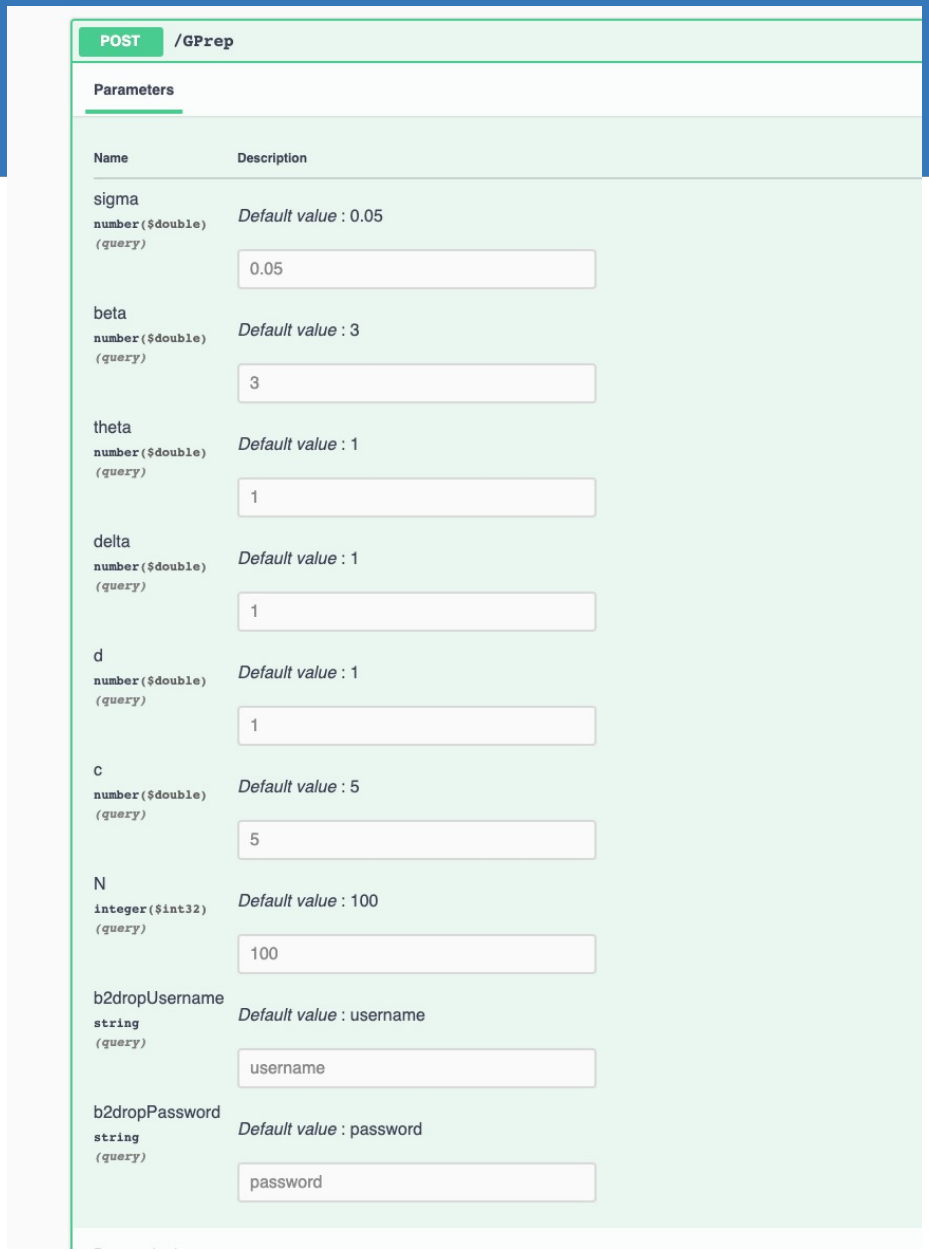
Gaussian API - Parameters

- **file** - reference data file from which the relevant forces and pair distances are extracted
  - **GPrep** method: user should upload the file
  - **GPrepRemote** method: user should provide public URL of the file (*default value: https://gaussian.chem-api.finki.ukim.mk/static/reference_data.xyz*)
- **sigma** - data noise standard deviation (*default value 0.05*)
- **beta** - exponential damping factor (*default value 3.0*)
- **theta** - latent function length scale (*default value 1.0*)
- **delta** - latent function standard deviation (*default value 1.0*)
- **d** - cutoff transition width (*default value 1.0*)
- **c** - cutoff (*default value = 5.0*)
- **N** - number of data points (*default value = 100*)
- **b2dropUsername** - **B2DROP** generated username – to upload the result files
- **b2dropPassword** - **B2DROP** generated password - to upload the result files

GPrep (POST method)

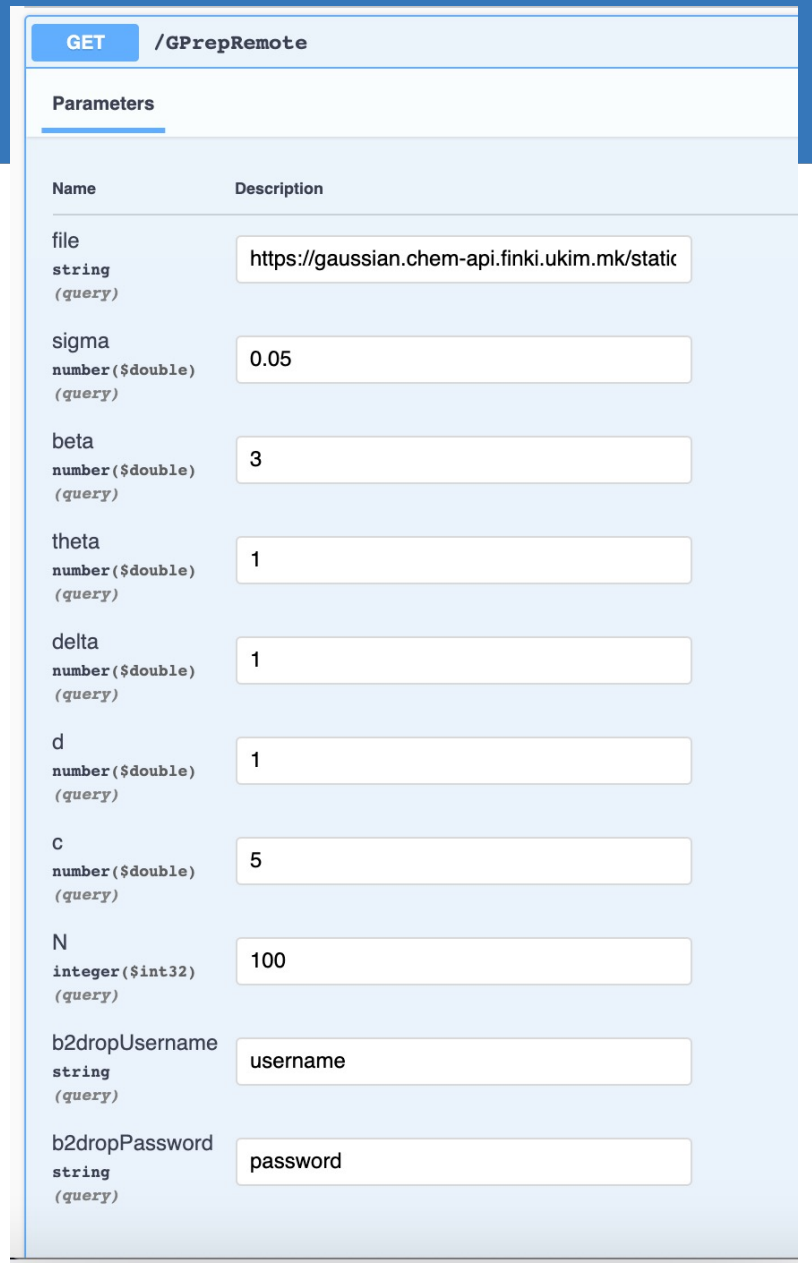
- Upload the input file directly on the Gaussian API home page





GPrepRemote (GET method)

- B2DROP username and password must be entered in the b2dropUsername and b2dropPassword textboxs in order to receive the output files (to be uploaded on the user's B2DROP account).



GPrepRemote (GET method)

- Other way to use this REST API method is to access it directly from the browser address bar.

  https://gaussian.chem-api.finki.ukim.mk/GPrepRemote?b2dropUsername=YOUR_B2DROPUSERNAME&b2dropPassword=YOUR_B2DROPPASSWORD&file=YOUR_FILE_LOCATION

- *If user preffers to change other paramerets, they can be added* as **&PARAMETER=VALUE**
- Another option is to consume this method in a program source code (Python)

```
import requests
response = requests.get('https://gaussian.chem-api.finki.ukim.mk/GPrepRemote?b2dropUsername=YOUR_B2DROPUSERNAME\
&b2dropPassword=YOUR_B2DROPPASSWORD&file=https://gaussian.chem-api.finki.ukim.mk/static/reference_data.xyz\
&sigma=0.05&beta=3.0&theta=1.0&delta=1.0&d=1.0&c=5.0&N=100')
if response.status_code == 200:
        print(response.content.decode('utf-8'))
else:
        print("None")
```

Service DEMO

- Gaussian Swagger link:

https://gaussian.chem-api.finki.ukim.mk/

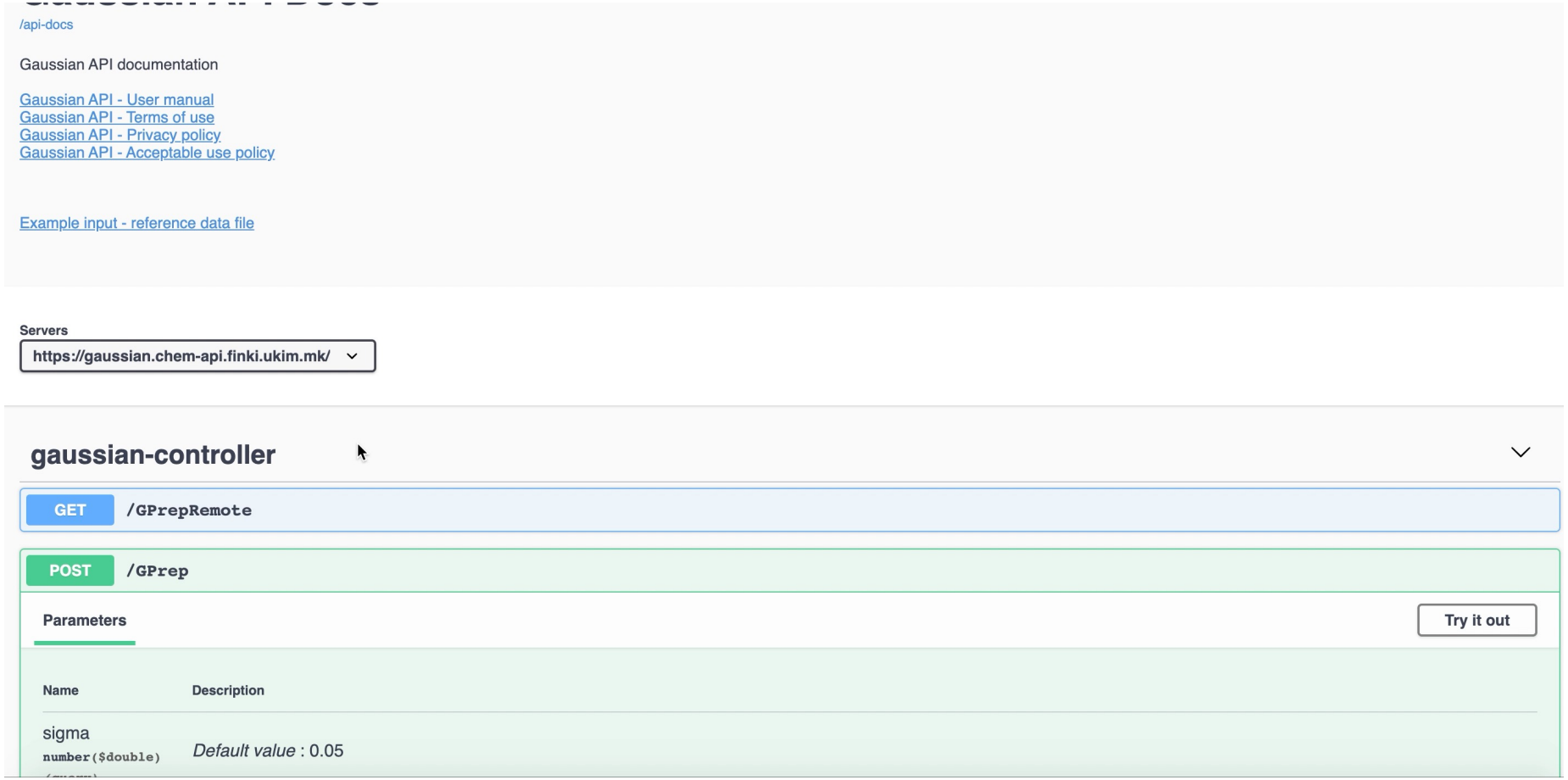
- Jupyter notebook link:

https://notebooks.finki.ukim.mk/user/user1/notebooks/GaussianAPI.ipynb

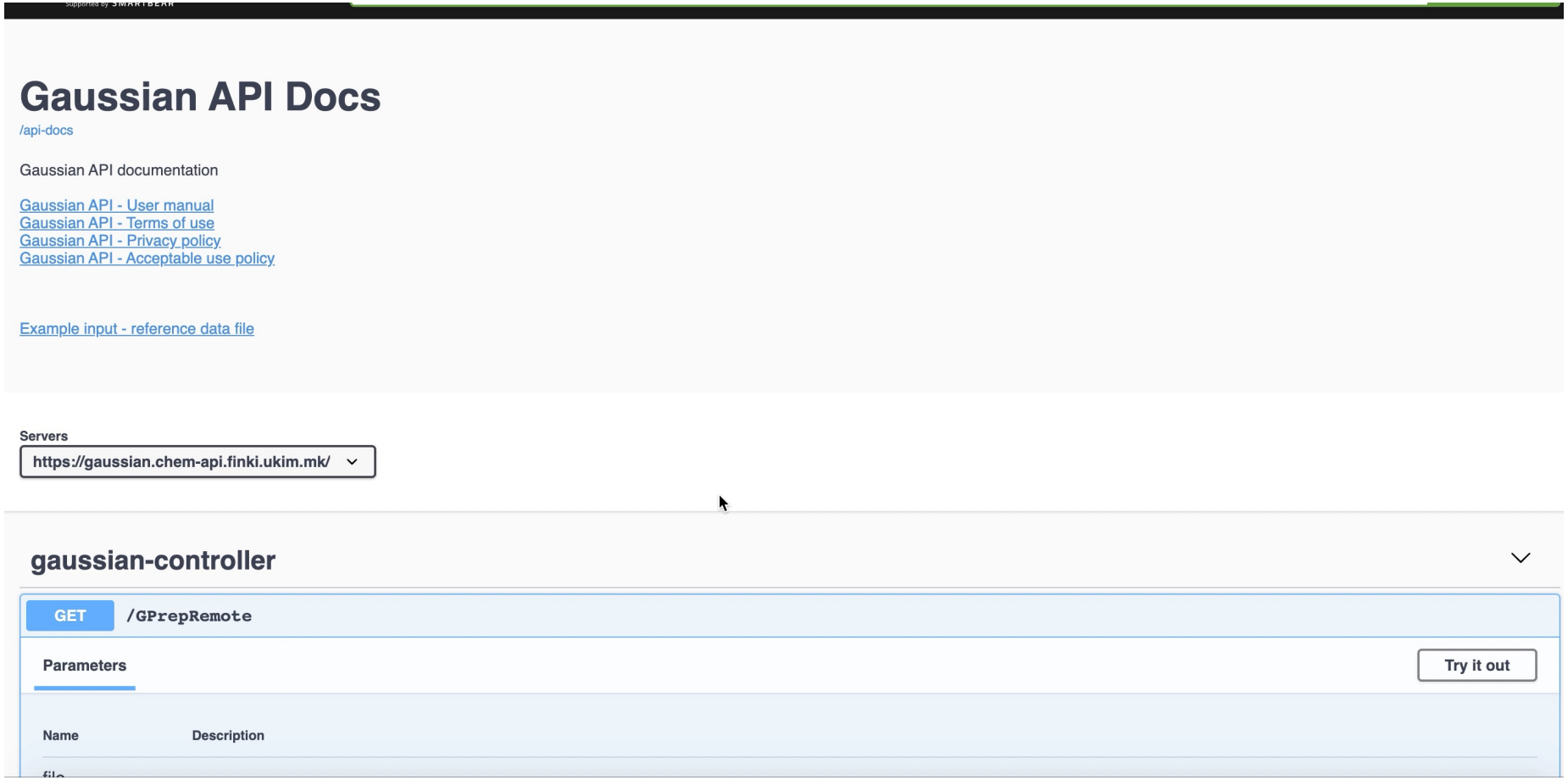
  - **User:** user1
  - **Password:** User1DEMO

The service demo videos can be seen on the next slides

Service DEMO - GPrep



Service DEMO - GPrepRemote



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