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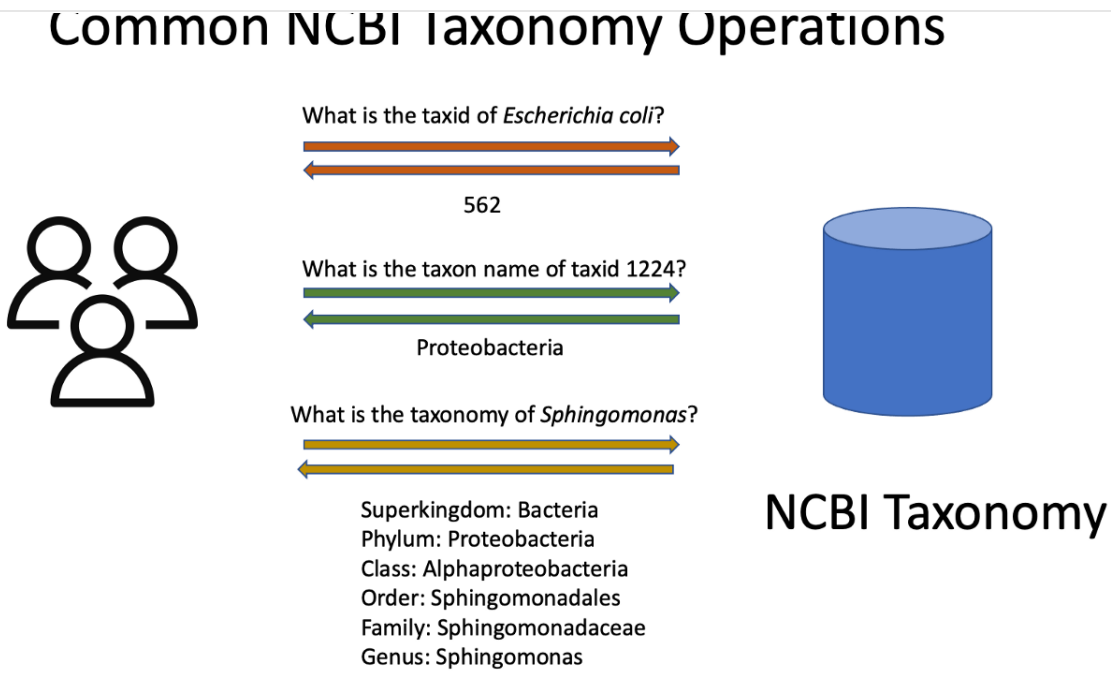
Serve NCBI Taxonomy in AWS, Serverlessly

Sixing Huang 1 day ago · 11 min read ★

The world is moving towards the cloud computing fast. This is because the cloud is very easy, cheap, accessible and secure. Cloud providers such as Amazon Web Service (AWS) take over many repetitive tedius IT maintenance tasks for their customers. As a result, cloud users can focus on their own business logics. The cloud also provide different pricing options that may be more cost effective than on-premises servers. In addition, unlike its on-premises counterparts, the cloud is very accessible and secure through the internet.

In this tutorial, I am going to show you how I managed a serverless NCBI taxonomy API service in AWS. In microbial bioinformatics, one of the most frequent tasks is the traverse of the NCBI taxonomy, because biologists needs to unambiguously define the taxonomic names in computer programs. This includes these operations: retrieving the scientific names, the taxonomic ranks, the parent taxa and the daughter taxa given a taxid and conversly, retrieving the taxid given a taxonomic name:



The problem: NCBI provides us with all this information in a group of text files, and they are not structured in an easily accessible way. The task is clear: to make this information programmatically accessible. And the access should be fast since these operations are performed very frequently.

Previously, I have written a blog post and a Python library Pyphy just for this purpose. Apart from my approach, there are other implementations out there in the Python world (etetoolkit, ncbi-taxonomist and taxadb). But some drawbacks comes to mind:

1. It is language specific. So the users need to write their programs in that language such as Python to make use of the libraries.
2. It is local. Whoever wants to use it, needs to set up the whole thing in their local environment. Each local copy needs updates individually afterwards. And you cannot access my installation via internet.
3. It scales poorly. Its performance depends on the hardware where it is installed. And there is no way to automatically scale it up when needed.

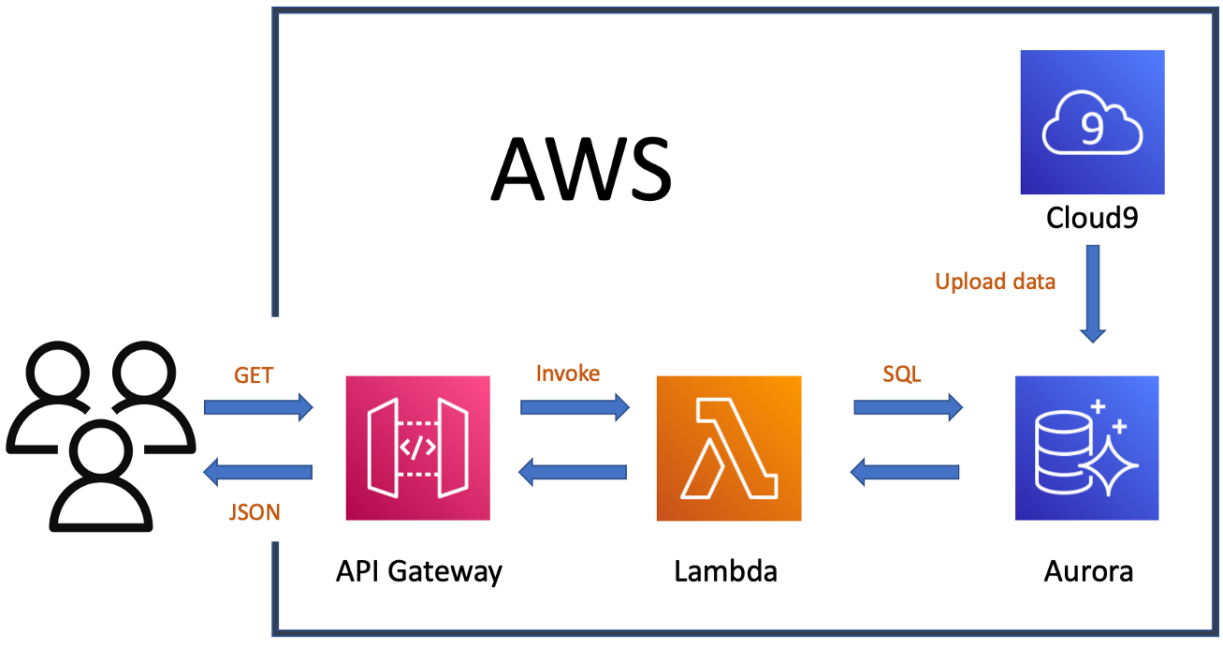
For this reason, I moved Pyphy into the AWS cloud and make it into a REST API service. It basically solves all the three drawbacks at once:

API, in fact, you can even just use an app like Postman or even a browser to interact.

2. It is on the cloud. As long as it is up and running, everybody with access to internet can use it right away without installing anything.
3. It scales. It is possible to set it up so that Amazon can increase the computation resources to meet the demand surge.

I have thought about various ways to make Pyphy onto AWS. But finally I settled onto the easiest and cheapest way:

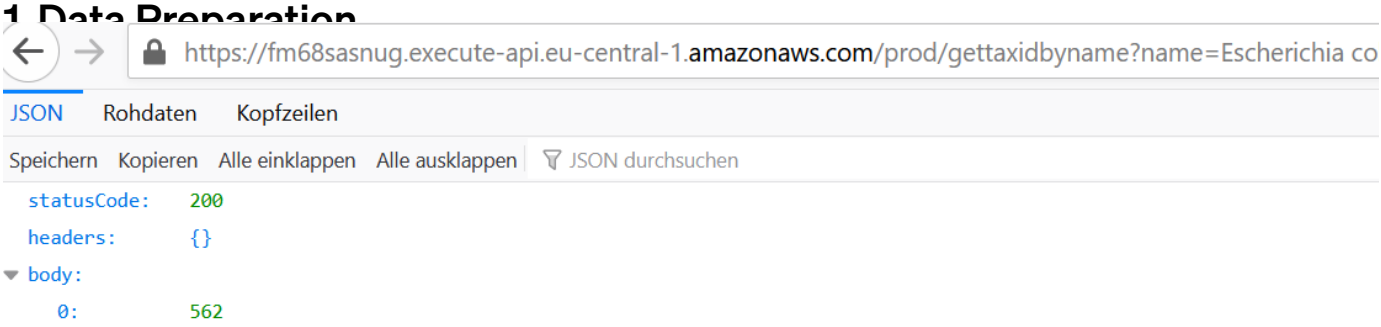
- Backend: Aurora serverless. I uploaded the data via a Cloud9 session.
- Frontend: API gateway with Lambda Function



Architect of the serverless NCBI taxonomy API

However, serverless Aurora skips a few calls after a certain period of inactiviy, because it needs to wake up after inactivity (the Stackoverflow discussion and solution is here). Therefore, if you need a persistent service, please consider using the provisioned Aurora.

1. Data Preparation

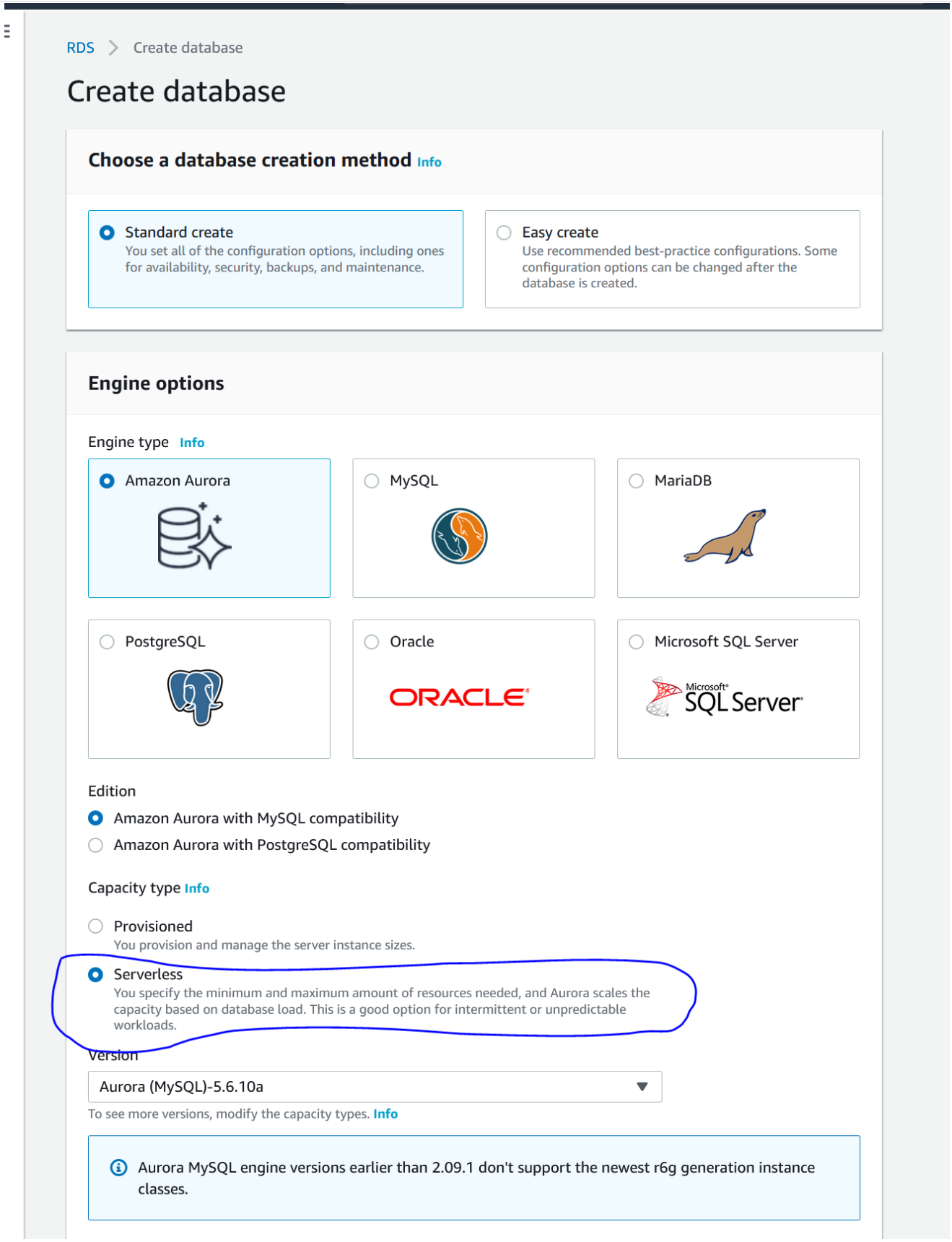


The code can be found in my Github repository here.

“synonym.tsv”. “tree.tsv” keeps the main information in one place, while “synonym.tsv” provides auxiliary information about the synonyms for some taxids. I accomplished this task with a Python script “prepyphy.py”. I finished this step on my local machine. Of course, you do it the “cloud native” way: upload the two “dmp” file and my “prepyphy.py” onto AWS Cloud9 and perform the same task.

2. Setup serverless Aurora

Now it is time to head to AWS. After logging into the AWS account, open Amazon RDS and create a severless Aurora: select the “Serverless” under “Capacity type”:

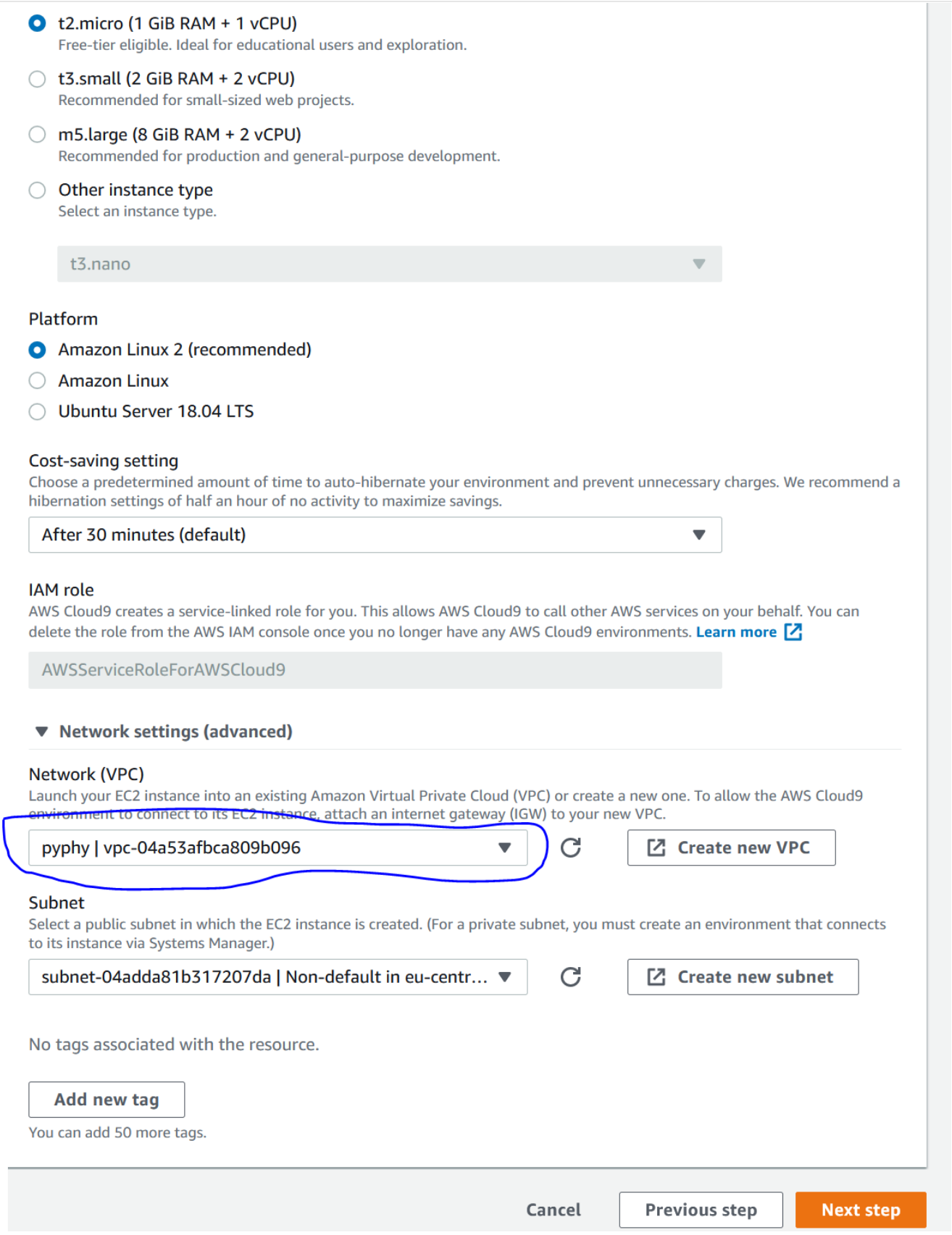

RDS > Create database
Create database
Choose a database creation method Info
Standard create
You set all of the configuration options, including ones for availability, security, backups, and maintenance.
Easy create
Use recommended best-practice configurations. Some configuration options can be changed after the database is created.
Engine options
Engine type Info
Amazon Aurora
MySQL
MariaDB
PostgreSQL
Oracle
Microsoft SQL Server
Edition
Amazon Aurora with MySQL compatibility
Amazon Aurora with PostgreSQL compatibility
Capacity type Info
Provisioned
You provision and manage the server instance sizes.
Serverless
You specify the minimum and maximum amount of resources needed, and Aurora scales the capacity based on database load. This is a good option for intermittent or unpredictable workloads.
Version
Aurora (MySQL)-5.6.10a
To see more versions, modify the capacity types. Info
Aurora MySQL engine versions earlier than 2.09.1 don't support the newest r6g generation instance classes.

password. This credential is necessary later for the data import.

As to “Connectivity”, create a new VPC “pyphy” for this tutorial. Under “Additional configuration”, please check “Data API” for debugging. All the other options and parameters are default. Click “Create database” to let AWS prepare the database.

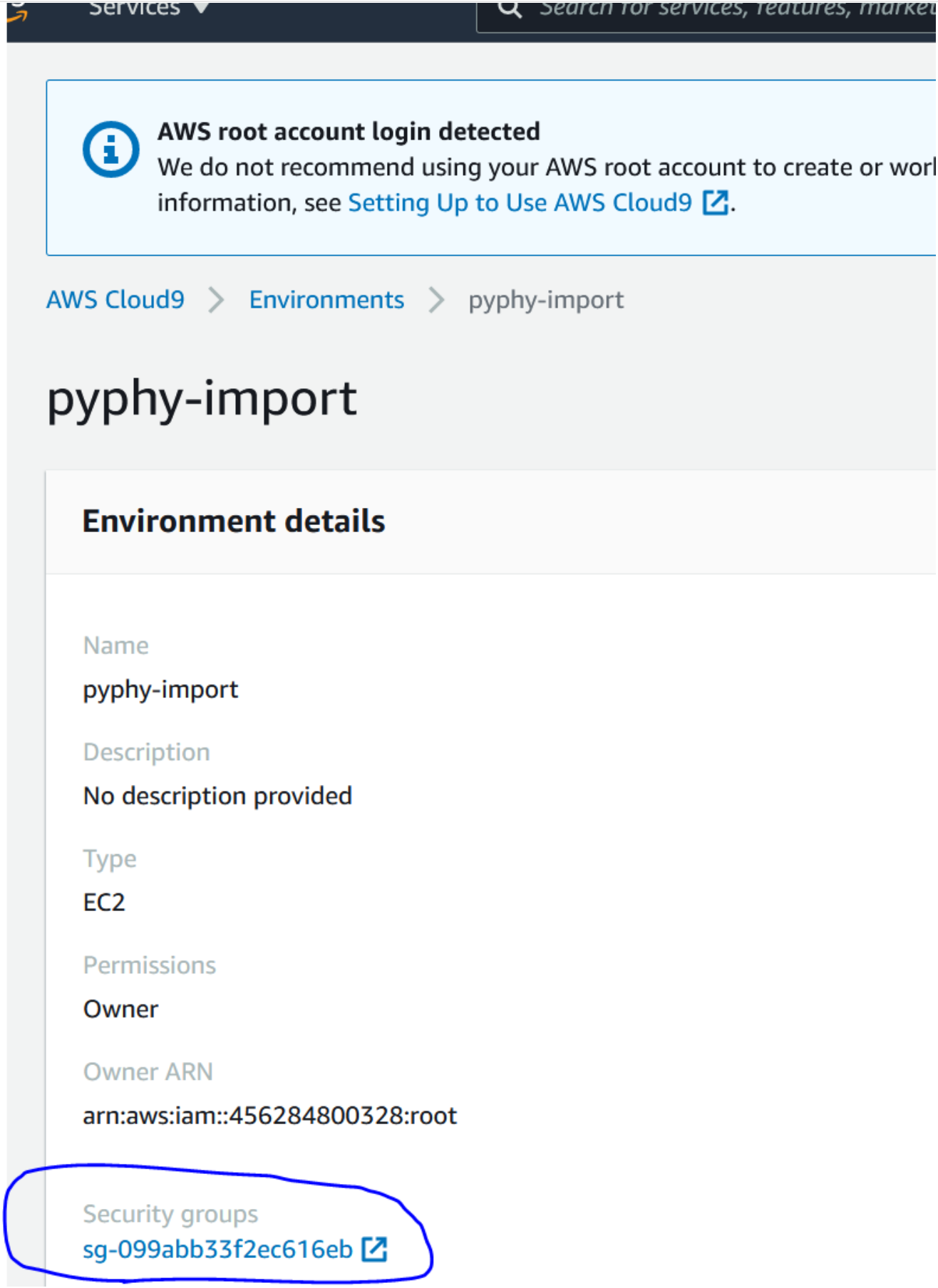
3. Import data into Aurora

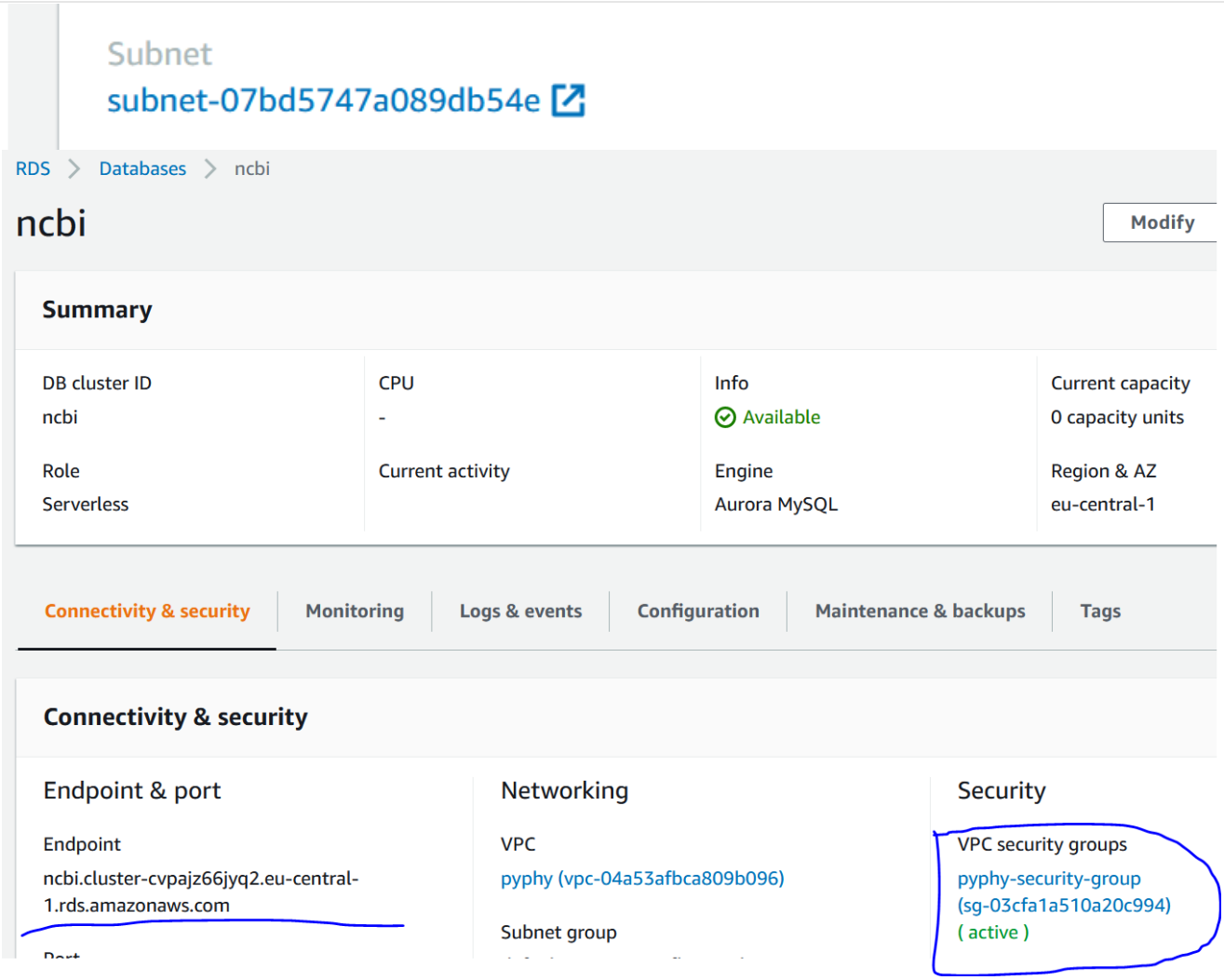
Now switch to Cloud9. Select the same region as our Aurora database. Start by clicking “Create environment” and name it as “pyphy-import”. In Step 2 “Configure settings”, unfold “Network settings (advance)” and choose the same VPC as our Aurora database. Then go on to finish creating the Cloud9 environment.



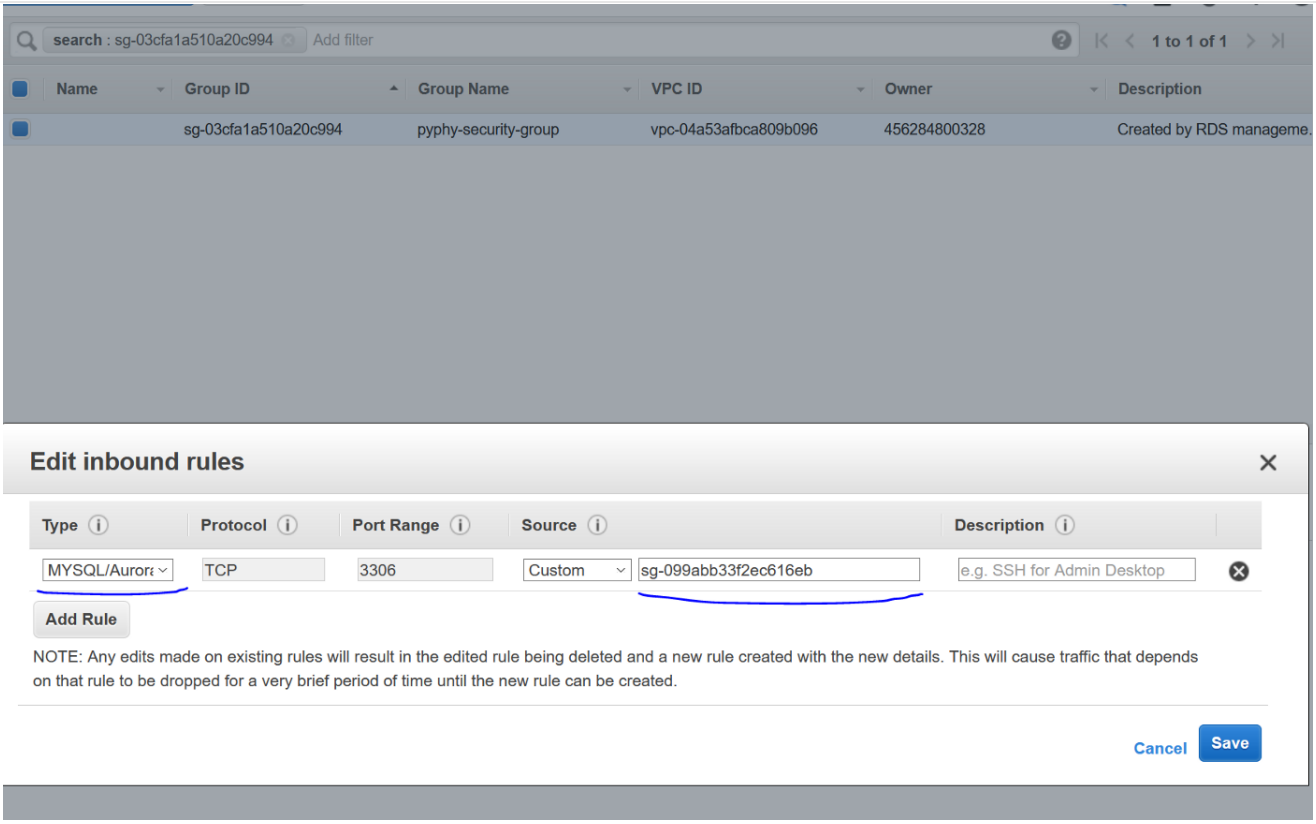
3.1. Allow connection bewteen Cloud9 and Aurora

of our newly created “pyphy-import” environment and copy the Security groups identifier.


Services
Search for services, features, marketplace
AWS root account login detected
We do not recommend using your AWS root account to create or work
information, see Setting Up to Use AWS Cloud9.
AWS Cloud9 > Environments > pyphy-import
pyphy-import
Environment details
Name
pyphy-import
Description
No description provided
Type
EC2
Permissions
Owner
Owner ARN
arn:aws:iam::456284800328:root
Security groups
sg-099abb33f2ec616eb



In the security group page, click “Inbound” and “Edit”, add a rule of type “MYSQL/Aurora”. In the “Source”, select “Custom” and paste the Cloud9 environment security group name into the text field.



3.2. Import tsv files into Aurora

Now we are ready for the data import. In our newly created Cloud9 environment, click “File -> Upload Local Files…” to upload both “synonym.tsv” and “tree.tsv”.

In the console panel in the lower half of the screen, we can use the normal mysql command to log into our Aurora database by:

```
mysql –h [database endpoint] –P 3306 –u [database master username]
–p
```

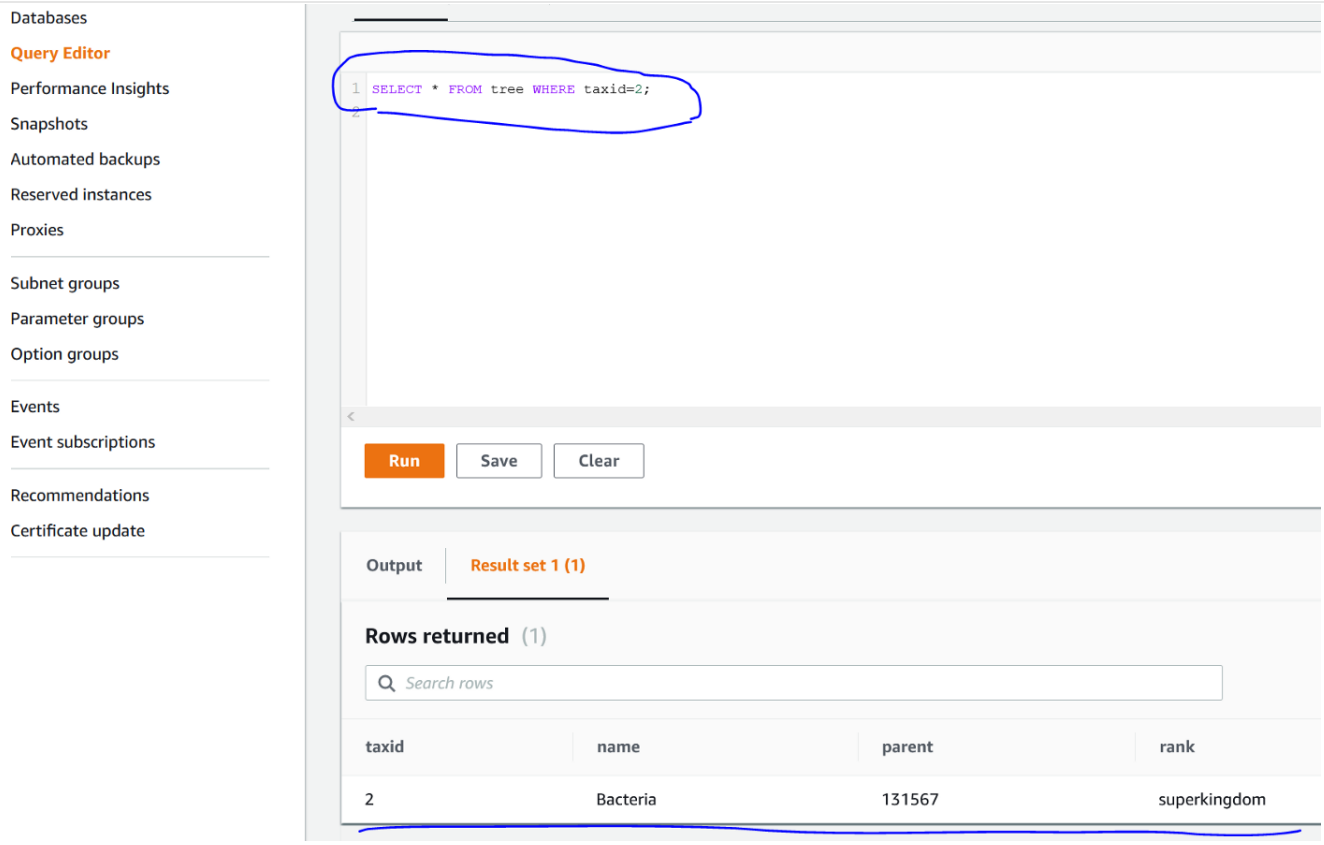
[database endpoint] is the URL that we wrote down in **3.1**. Master username is the one that we set when we created the Aurora database in **2**. This command will then ask for the master password from Step **2**. Once logged in, we can issue a series of commands to set up a database “pyphydb”. Inside it, we can import and index two tables: “tree” and “synonym”.

```
CREATE DATABASE pyphydb;

use pyphydb;

CREATE TABLE tree (taxid integer, name varchar(250), parent integer,
rank varchar(20));

CREATE TABLE synonym (id integer, taxid integer, name varchar(250));

load data local infile 'tree.tsv' into table tree fields terminated
by '\t' lines terminated by '\n' (taxid, name, parent, rank);

load data local infile 'synonym.tsv' into table synonym fields
terminated by '\t' lines terminated by '\n' (id, taxid, name);

CREATE UNIQUE INDEX taxid_on_tree ON tree(taxid);

CREATE INDEX name_on_tree ON tree(name);

CREATE INDEX name_on_synonym ON synonym(name);

CREATE INDEX taxid_on_synonym ON synonym(taxid);
```

Once done, we can check whether everything is OK back in Amazon RDS by issuing a query in "Query Editor". In "Connect to database" popup, enter the DB cluster name "ncbi", master username and password, and the database name "pyphydb". Be aware that it may take some minutes until serverless Aurora is set up. Once inside, issue a simple SQL

```
SELECT * FROM tree WHERE taxid=2;
```

to confirm that the data are imported properly:



4. Setup AWS Lambda

With the backend database done, it is time to move onto the frontend. Our frontend consists of two AWS components: Lambda Function and API Gateway. The latter takes care of the URL handling. And Lambda takes care of the querying of our Aurora database. To understand this, imagine that Alice and Bob both work in a baker shop. Alice stands in the front and takes orders from the customers. She then gives a concise message to Bob, who goes to the storage and fetches the bread to Alice. And Alice hands over the bread to the customers. In our case, Alice is the API Gateway and Bob is the Lambda Function. The storage is the Aurora database.

Currently, there are some gotchas in working with Lambda Functions in AWS. In our case, we need the Python library “pymysql” to interact with our Aurora database. But I could not find a way to install it in Lambda web editor. Instead, I need to create a deployment package (the files are also in my repository) and upload it to Lambda.

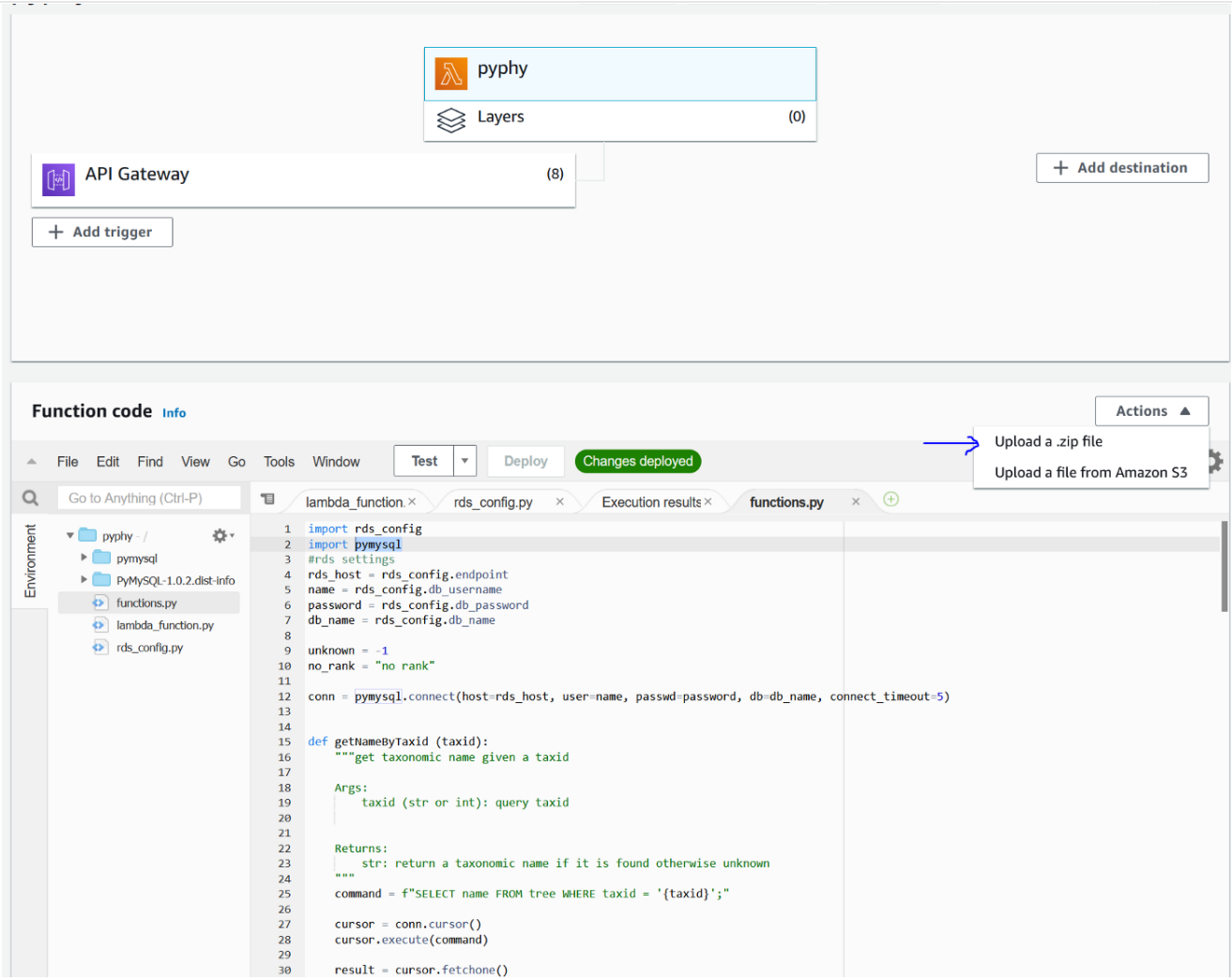
To do this, I created a folder in my local machine and installed the “pymysql” in it by issuing:

```
pip install PyMySQL -t .
```

Afterwards, I wrote three Python scripts. “functions.py” takes care of the SQL queries and returns the desired outputs. “lambda_function.py” will handle the messages from API gateway and route the requests to the correct functions. And “rds_config.py” stores the database credential. Remember to enter all the database credentials in “rds_config.py”. Zip these files in the folder level (do not zip the folder). Call it deployment.zip.

Now in Lambda, click “Create function” -> “Author from scratch”. Enter a function name such as “pyphy” and under “Runtime” select “Python 3.8”. Under “Advanced settings”, choose the same VPC and the same security group as our Cloud9 environment.

Once inside Lambda’s editor, click “Actions” -> “Upload a .zip file” to upload the deployment.zip. After a short while, you can see the code in main area. Make sure that the Handler is “lambda_function.lambda_handler” in the “Runtime settings”. Click the orange “Deploy” button to make the “pyphy” Lambda function online.



5. Setup AWS API Gateway

First off, I have structured my API URL as such:

```
method?field=identifier
```

For example, in order to get the taxid of “Flavobacteriia”, I can issue the following query URL:

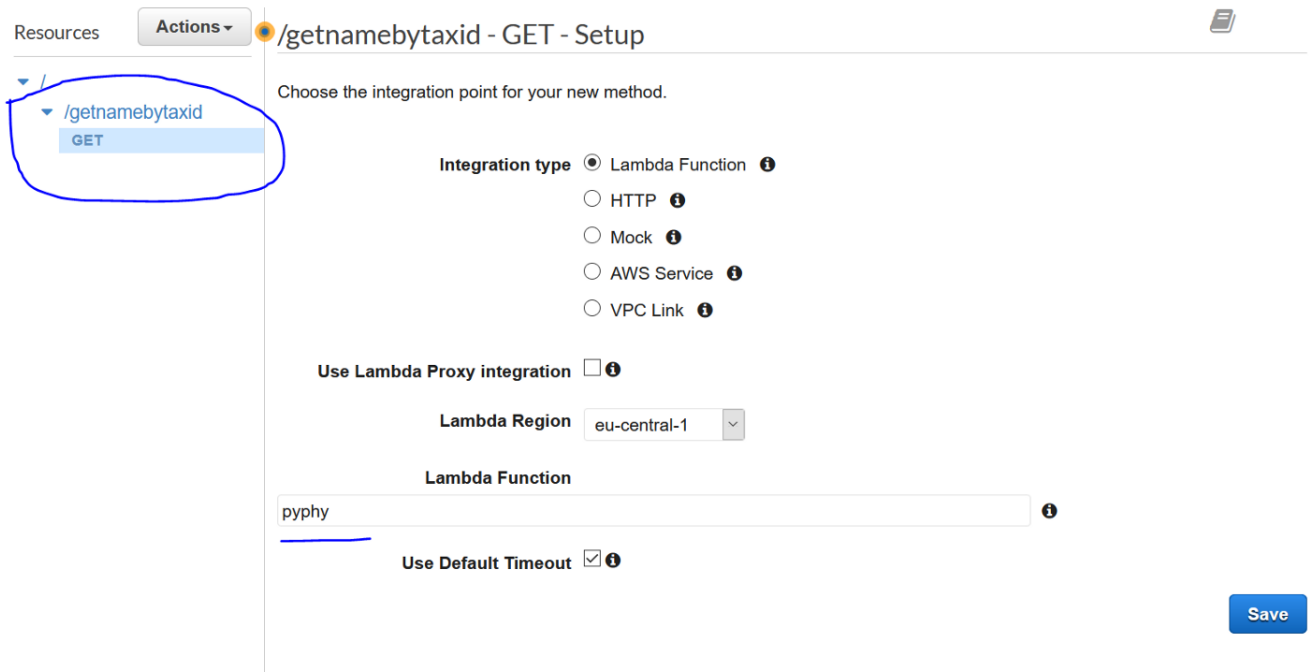
```
https://[api_gateway_invoke_URL]/gettaxidbyname?name=Flavobacteriia
```

be sufficient to take care of the most commonly used NCBI taxonomy operations. Except the method “gettaxidbyname” that requires an the field of “name”, all the other five functions require a field of “taxid”.

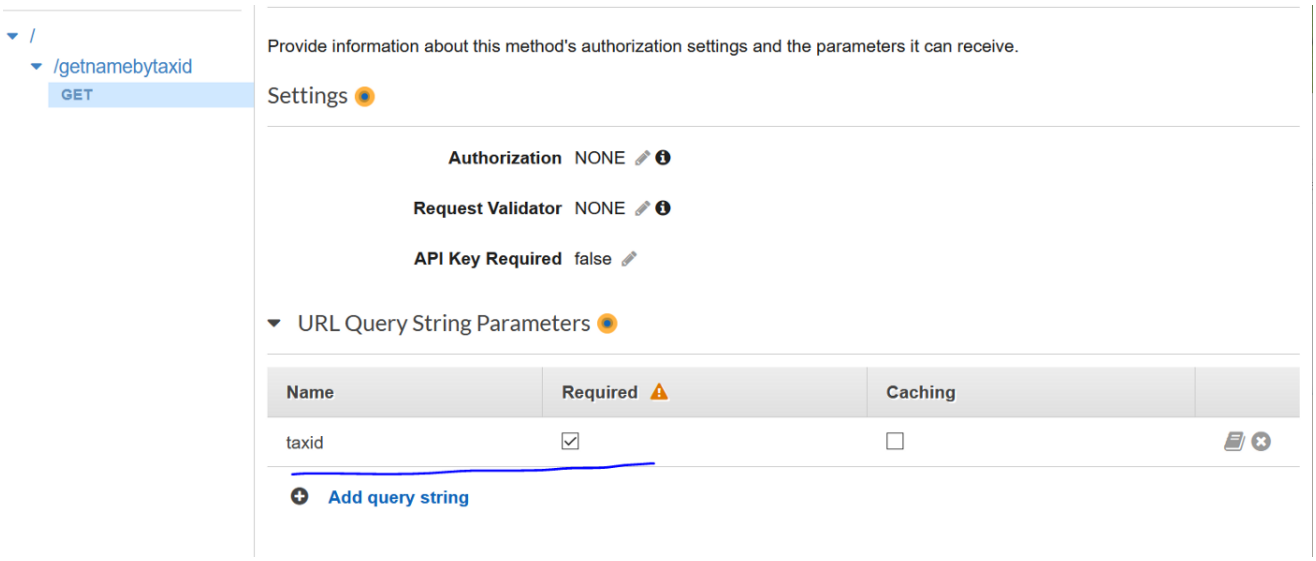
We need to define these in API Gateway. In the API Gateway page, click “Create API”. Click the orange “Build” button in the third “REST API” (not the “Private” one). Make sure “New API” is selected and give the API a name like “pyphy”.

5.1 Create the first resource and its GET method

Once created, we are onto the API editor page. Click the “Actions” dropdown and click “Create Resource”. In “Resource Name*”, enter our first method name “getnamebytaxid”, click “Create Resource”. When “/getnamebytaxid” is highlighted, click “Actions” dropdown again and click “Create Method”. A small dropdown will appear beneath our “/getnamebytaxid” resource. Open that small dropdown and select “GET” and click the small “check” icon to confirm. On the right side panel, a setup page appears. Make sure “Integration type” is “Lambda Function”. In “Lambda Function” input field enter “pyphy” (a hint dropdown should show up and let us auto-complete it). Click “Save”.



Now the “Method Execution” panel appears. Click “Method Request” on the first box.



Return to “Method Execution” by clicking “← Method Execution”. Now click “Integration Request” and unfold “Mapping Templates”. Choose “When there are no templates defined (recommended)”. Click “Add mapping template” and enter “application/json” and click the small “check” icon to confirm. A text box will appear below. Enter and save:

AWS Lambda Aws Api Gateway Aws Aurora AWS Ncbi

```
{
 “method”: “$context.resourcePath”,
 “taxid”: “$input.params(‘taxid’)”
}
```

This concludes the configuration of “/getnamebytaxid”.

5.2 Repeat the same for the other four “bytaxid” resources

Now we can set up the other four “bytaxid” resources “/getdictpathbytaxid”, “/ xid” and “/getsonsbytaxid”. The procedures are .

5.3 Add the final resource

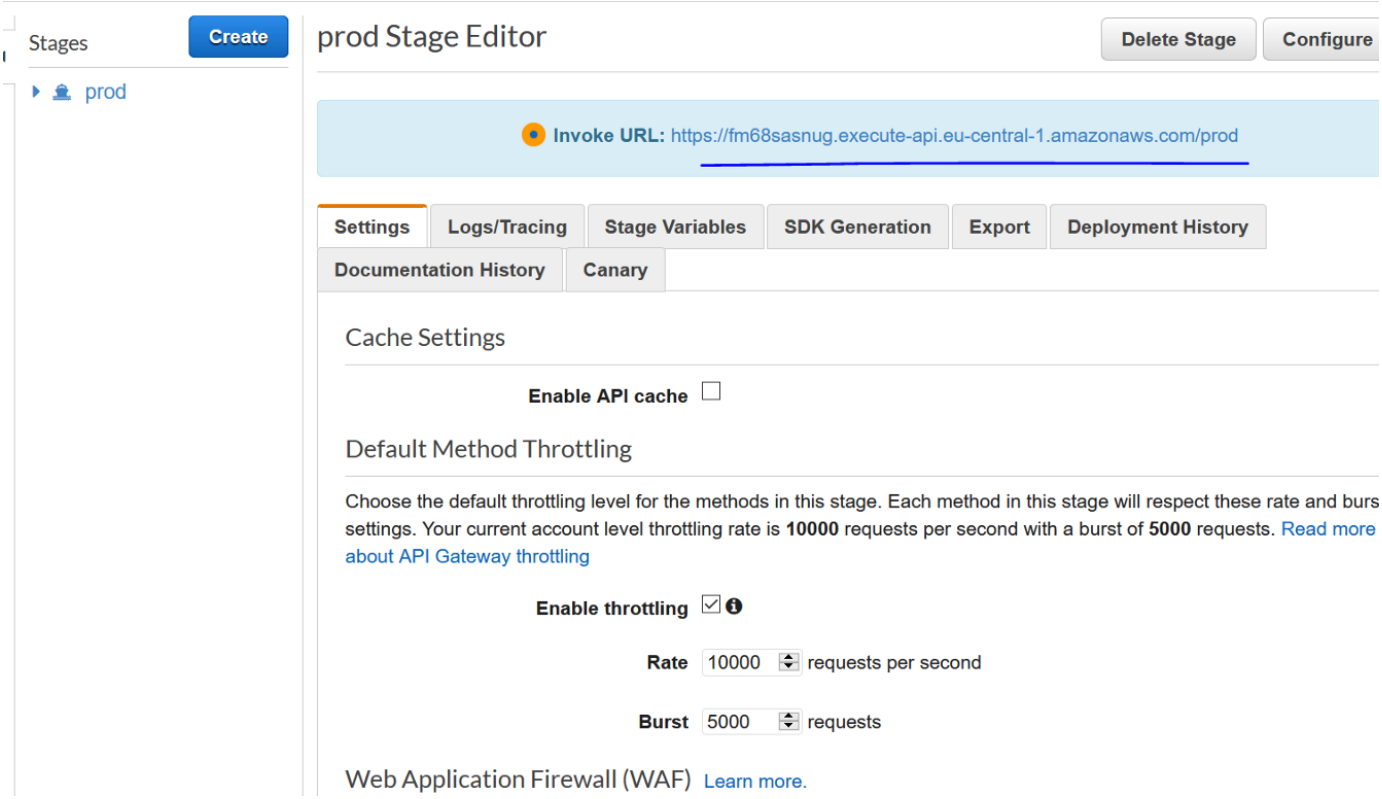
The last resource “/gettaxidbyname” requires a “name” input field. Its setup is nearly identical to those above and it only differs in:

2. in “Mapping Templates” under “Integration Request”, the text box should be:

```
{
 “method”: “$context.resourcePath”,
 “name”: “$input.params(‘name’)”
}
```

5.4 Deploy the API

Now it is time to deploy the API. Click “Actions” and click “Deploy API”. In the popup, enter “prod” as Deployment stage and click “Deploy”. This will lead to a new page in the right panel Under “Invoke URL”, we can find our individual URL endpoint.



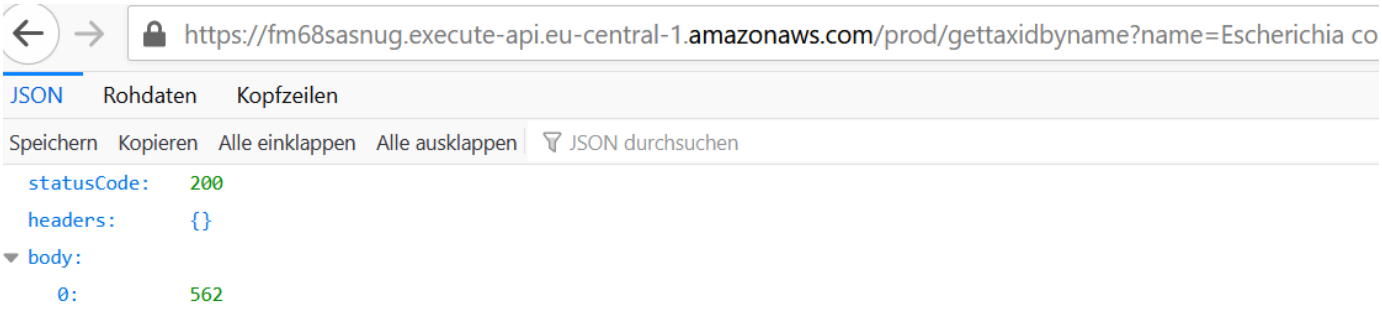
5.5 Test the API

Now let’s test whether the API works.

1. Get the taxid of “Escherichia coli” by issuing:

https://[your Invoke URL]/prod/gettaxidbyname?name=Escherichia%20coli

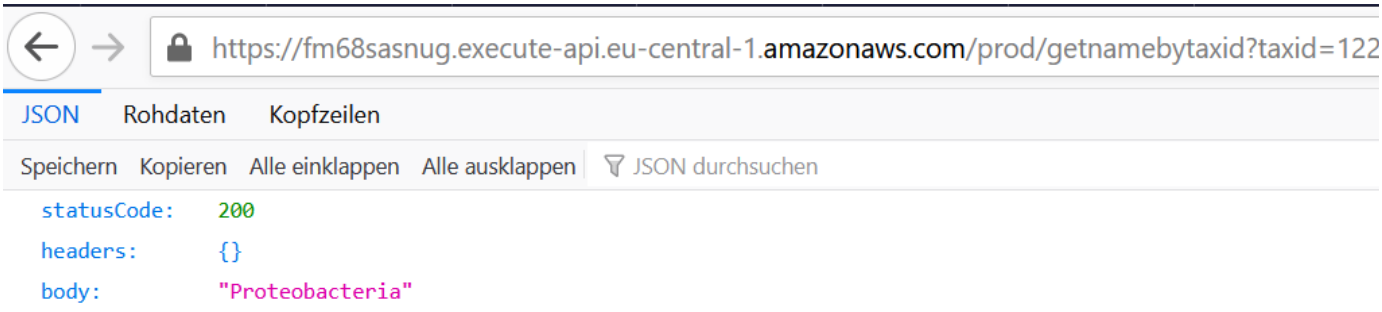
And I got back “562” in the body section:



2. Get the name of taxid 1224 by issuing:

https://[your Invoke URL]/prod/getnamebytaxid?taxid=1224

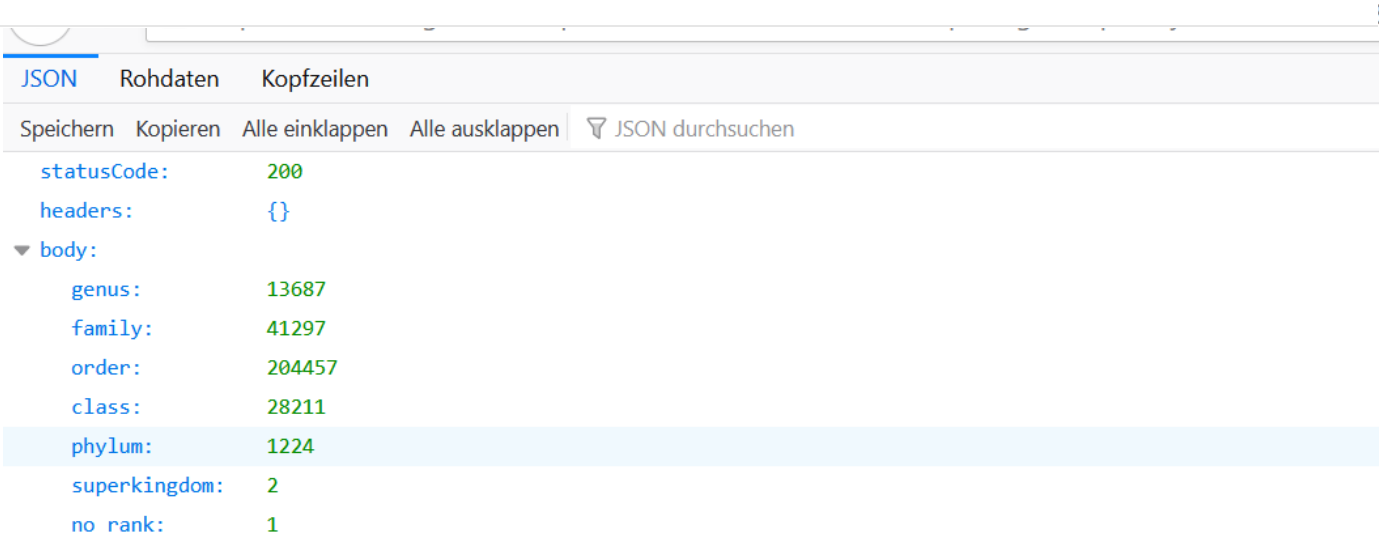
And I got “Proteobacteria”:



3. Get the taxonomic path for Sphingomonas (taxid 13687) by issuing

https://[your Invoke URL]/prod/getdictpathbytaxid?taxid=13687

And I got back:



6. Conclusion

Success! Now we have an online API that can serve the whole world with NCBI taxonomy. It is language agnostic, scalable and easy to use. It is also relatively easy to maintain: just upload t newer version of tree.tsv and synonym.tsv and it is done.

Certainly, there are other ways to achieve the same goal in AWS. For example, I can think of u the Application Load Balancer to distribute the input traffic to Fargate that queries the Aurora database with node.js. Maybe I can get rid of Aurora and run a fleet of nodes orchestrated by EKS.

This tutorial shows the hard way to set up the whole thing. I am now planning to summarize t tutorial in Terraform, so that the whole infrastructure can be set up in a heartbeat. Also, other tools such as Ansible and Chef may also come into play for configuring the database. The learning possibility in such a project is truely endless.

Now, it is your turn to use your creativity to show me some interesting AWS projects!