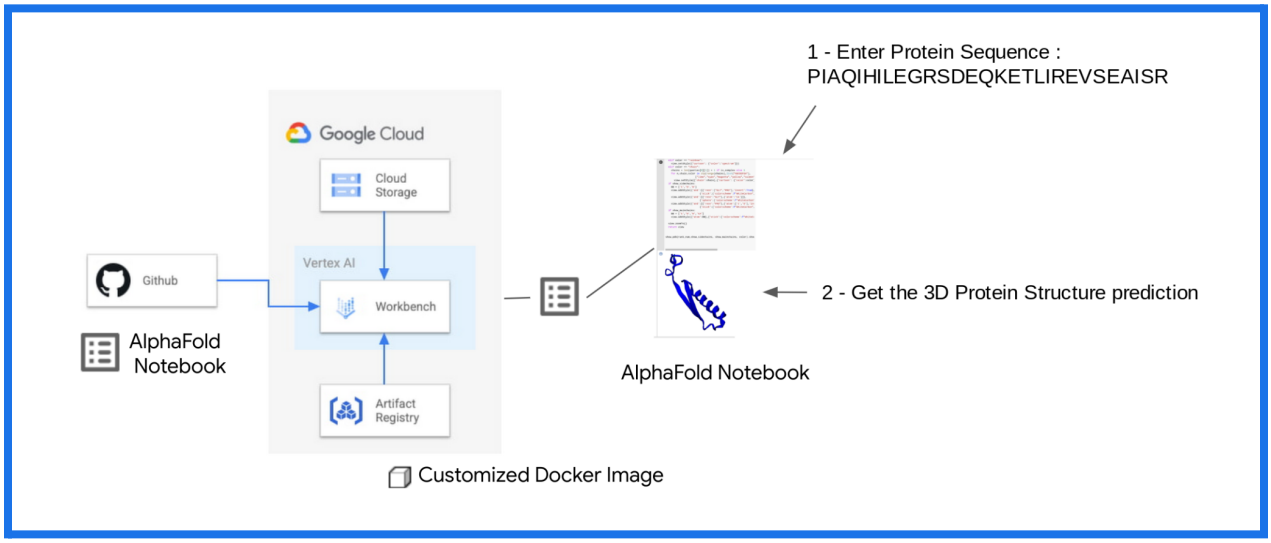
Hands on AlphaFold with Vertex AI

4th August 2022

Alphafold is Deepmind's Machine Learning based protein structure prediction system.
Within this hands-on session we will walk through a demonstration notebook that can predict the structure of a protein using a slightly simplified version of AlphaFold that does not use homologous protein structures or the full-sized BFD sequence database.
Please note that this session is provided as an early-access prototype and is not reflecting the quality of a finished product. It is provided for theoretical modeling only and caution should be exercised in its use.

Hands On Overview:



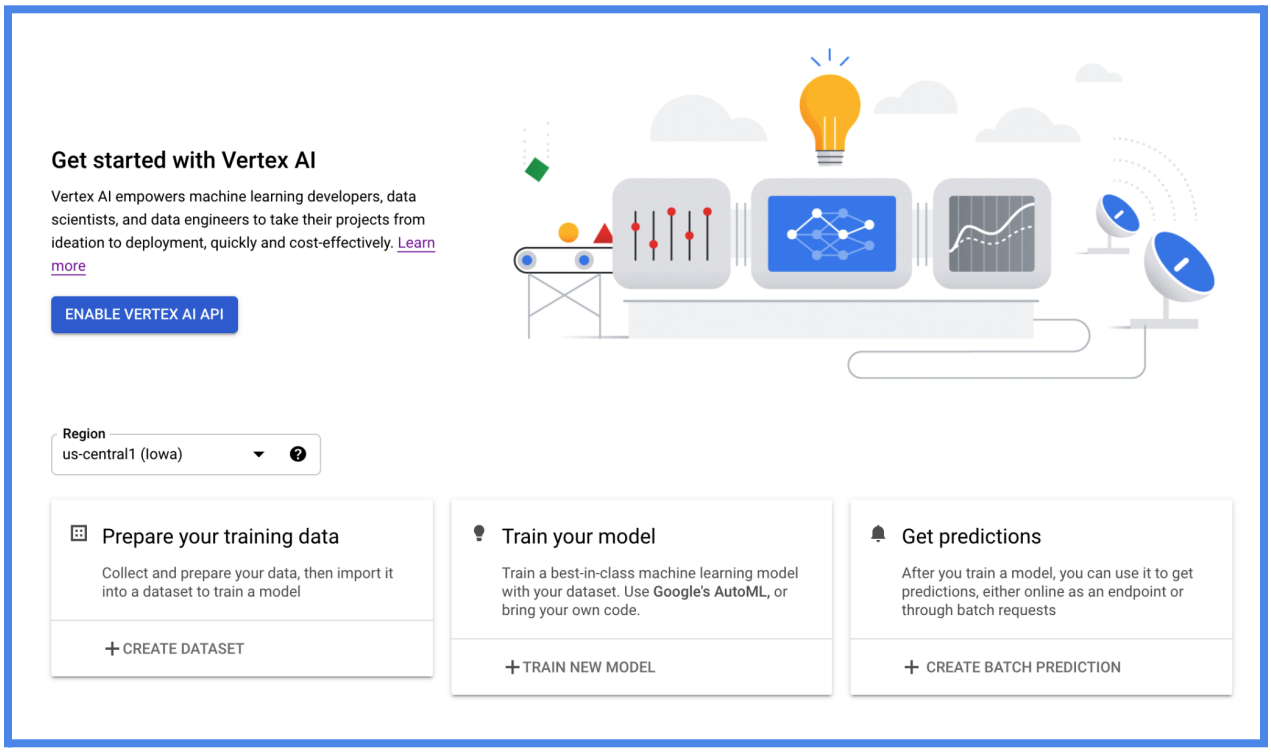
[1] Open a new incognito tab and open this guide in the incognito session

[2] Go to: https://console.cloud.google.com/

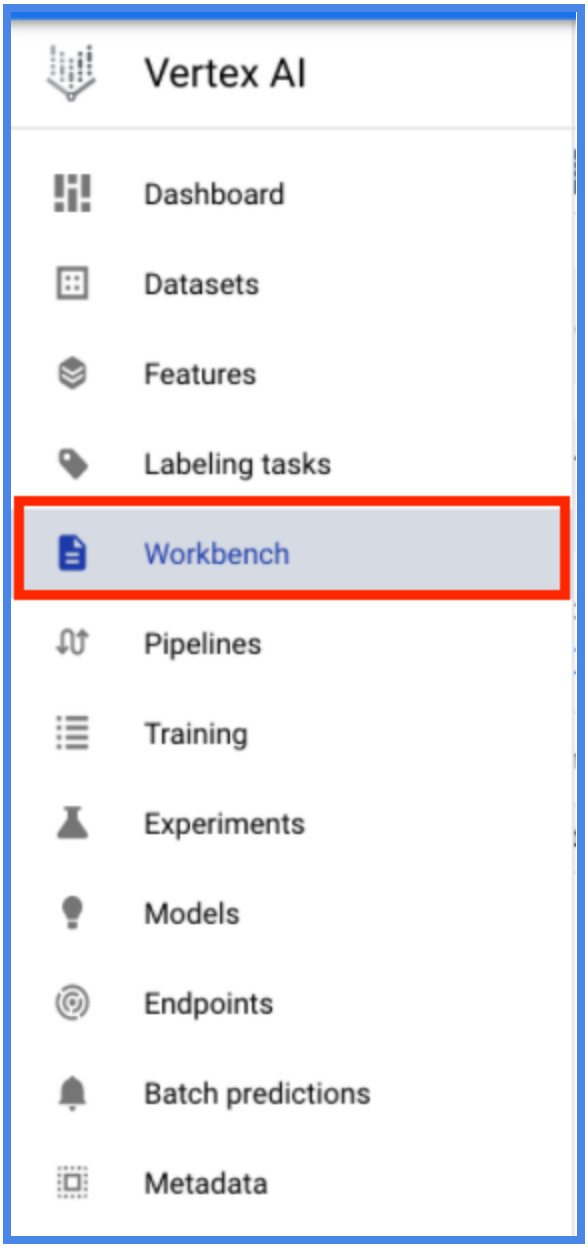
[3] Connect with the provided credentials
[3.1] Ensure you select the "project" by selecting it in the top blue bar drop down menu

[4] Enable APIs first, in the top head search bar, search Vertex AI , then click on Vertex AI:

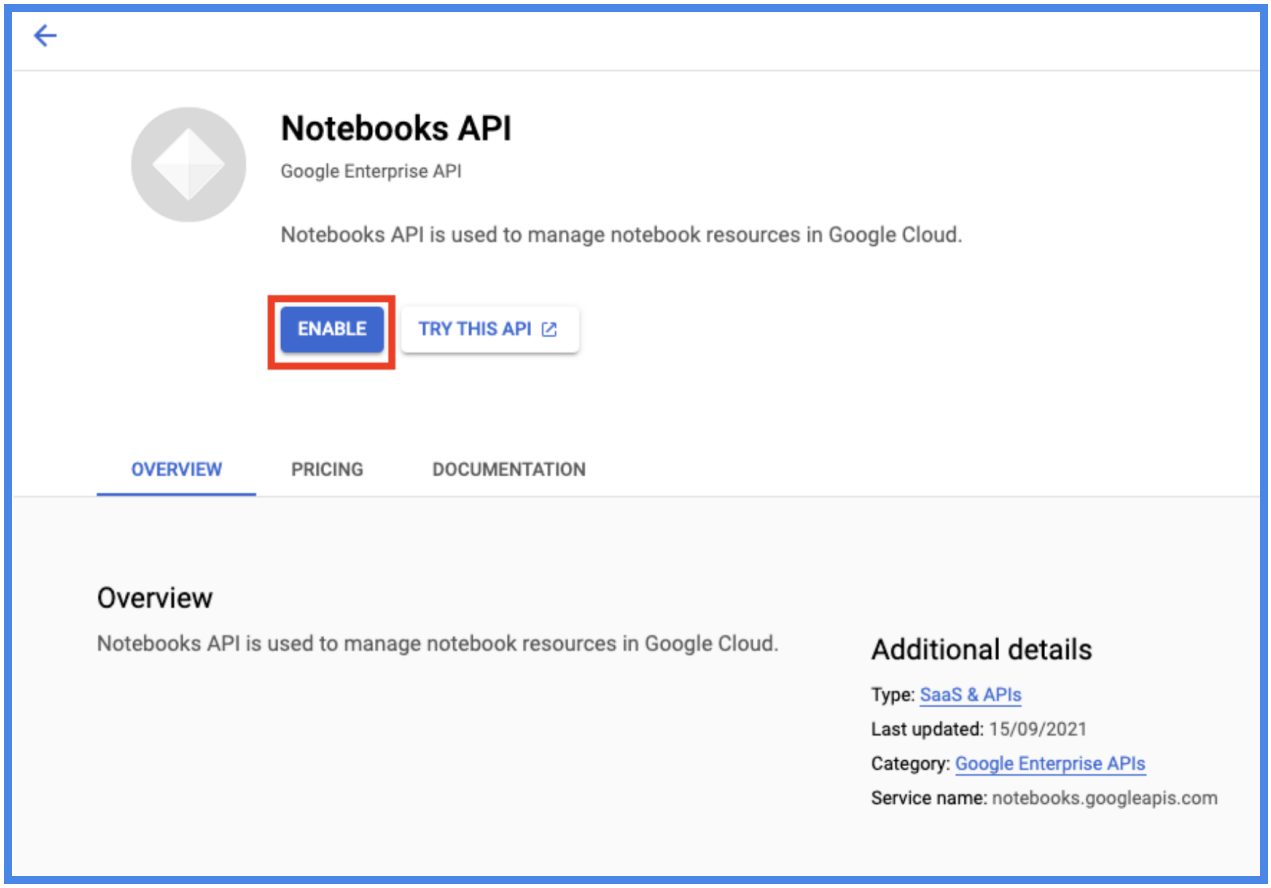
[5] Click the **Enable VERTEX AI API** button



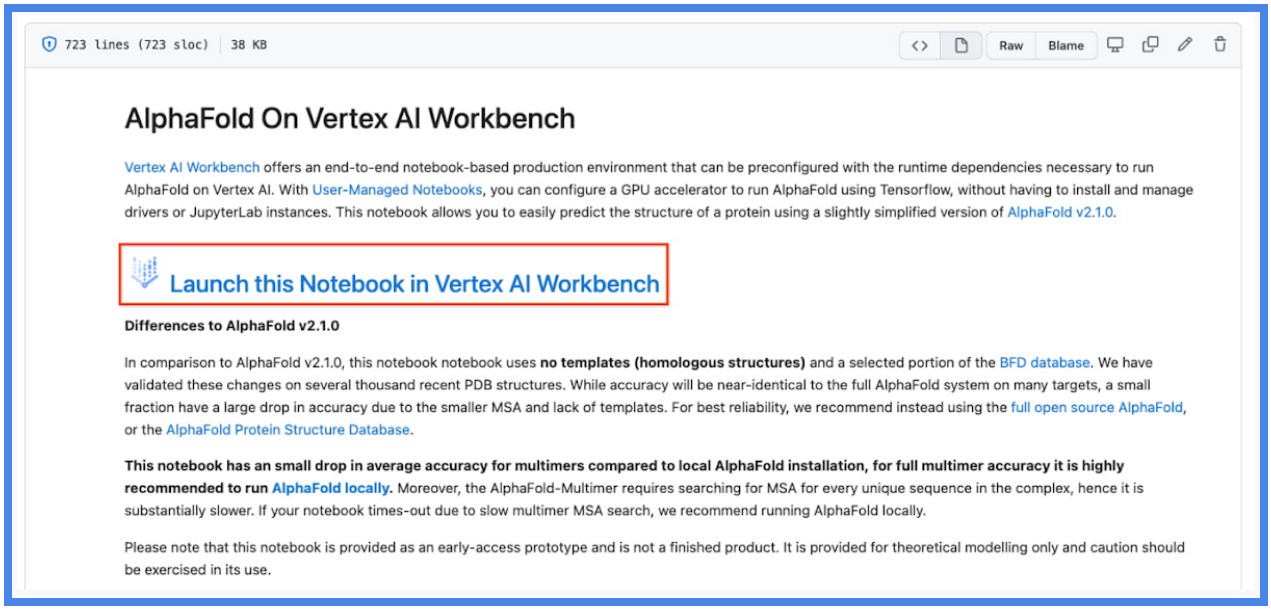
[6] On the left side Navigate in Workbench:



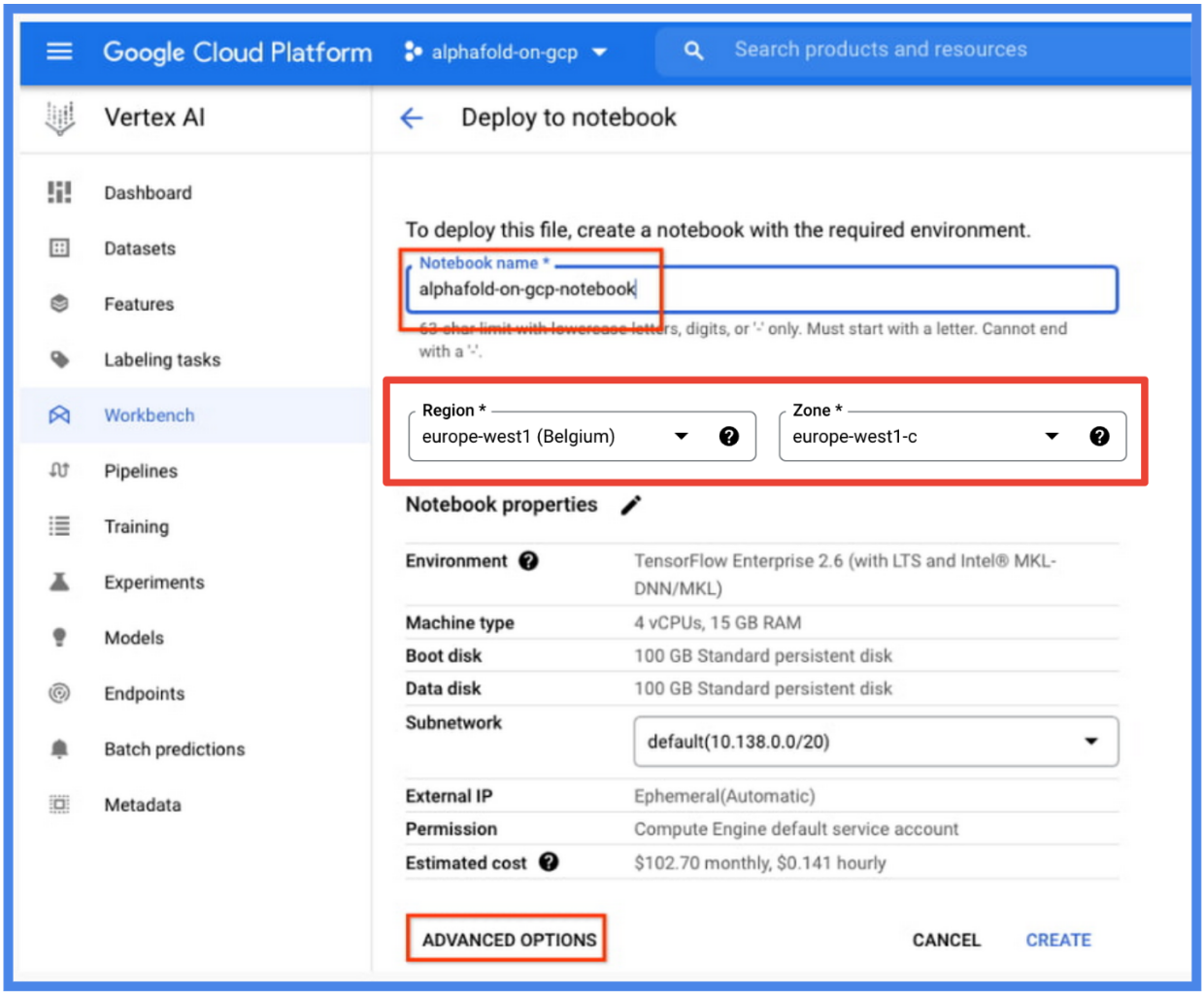
[7] Enable the NotebookAPI by clicking the **Enable** button



[8] Get the Notebook by visiting :
https://github.com/GoogleCloudPlatform/vertex-ai-samples/blob/main/community-content/alphafold_on_workbench/AlphaFold.ipynb



[9] Continue the Notebook creation Selecting a Name typing it in the **Notebook name** section, select **Europe West 1** as Region and **don't click "Create" just yet** :



[10] Click **ADVANCED OPTIONS** section

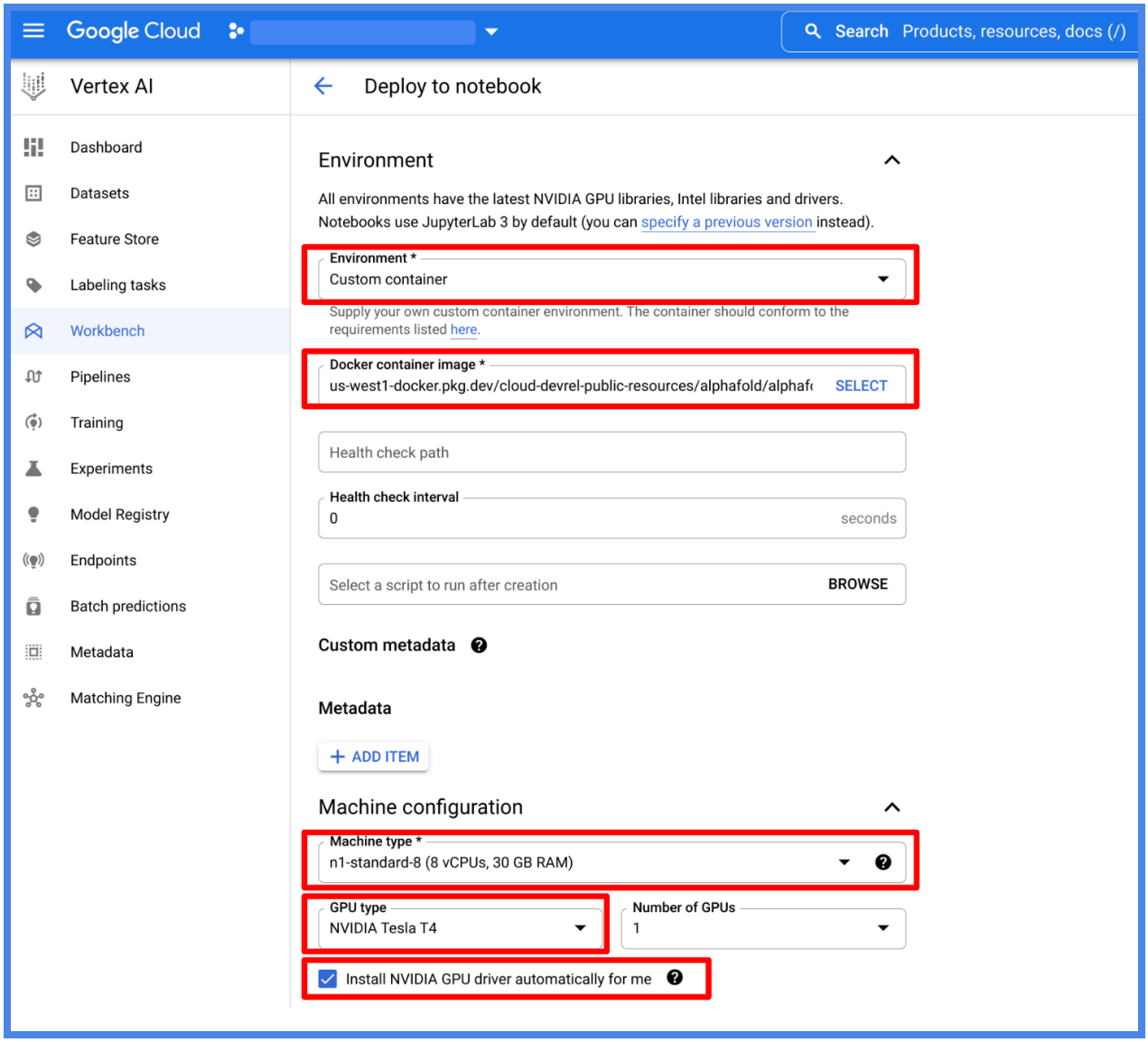
[11] Select **Custom container** in the **Environment** drop down from the **Environment** section

[12] In the “Docker container image” text box, enter (without clicking “select”):
`us-west1-docker.pkg.dev/cloud-devrel-public-resources/alphafold/alphafold-on-gcp:latest`

[13] Machine type drop down : Machine type: n1-standard-8 (8 CPUs, 30 GB RAM)

[14] GPU Type drop down : NVIDIA Tesla T4

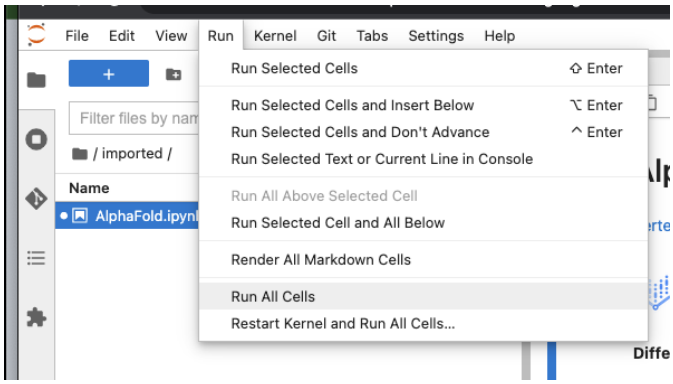
[15] check box “Install NVIDIA GPU driver automatically for me“



[16] Press **Create** !

[17] After several minutes, a virtual machine will be created and you will be redirected to a JupyterLab instance. When launching, you may need to confirm the connection to the Jupyter server running on the VM; click the `Confirm` button

[18] The notebook is ready to run! From the menu, select **Run > Run all Cells** to evaluate the notebook top-to-bottom, or run each cell by individually highlighting and clicking **<shift>-return**. The notebook has detailed instructions for every step, such as where to add the sequence(s) of a protein you want to fold.



[19] Congratulations, you've just folded a protein using AlphaFold on the Vertex AI Workbench!