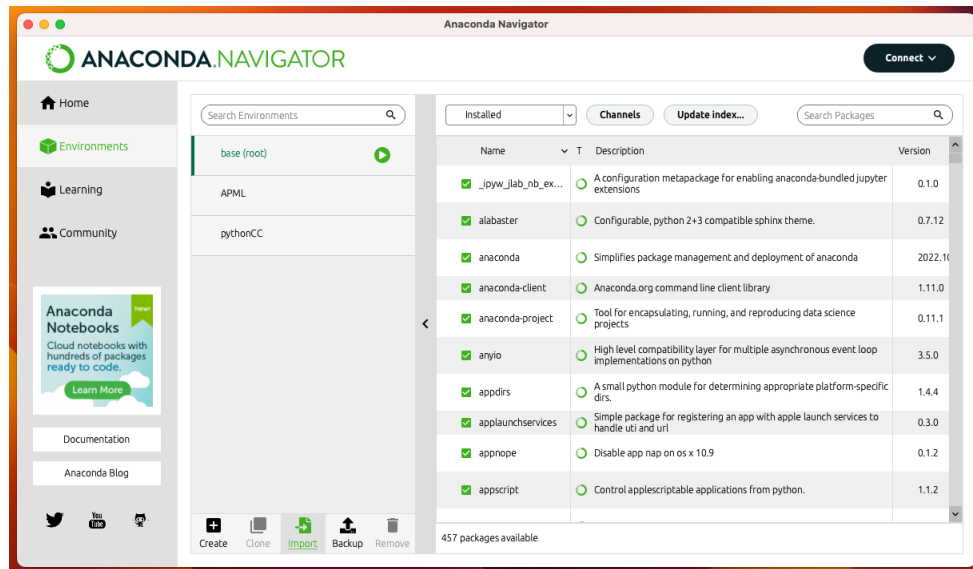
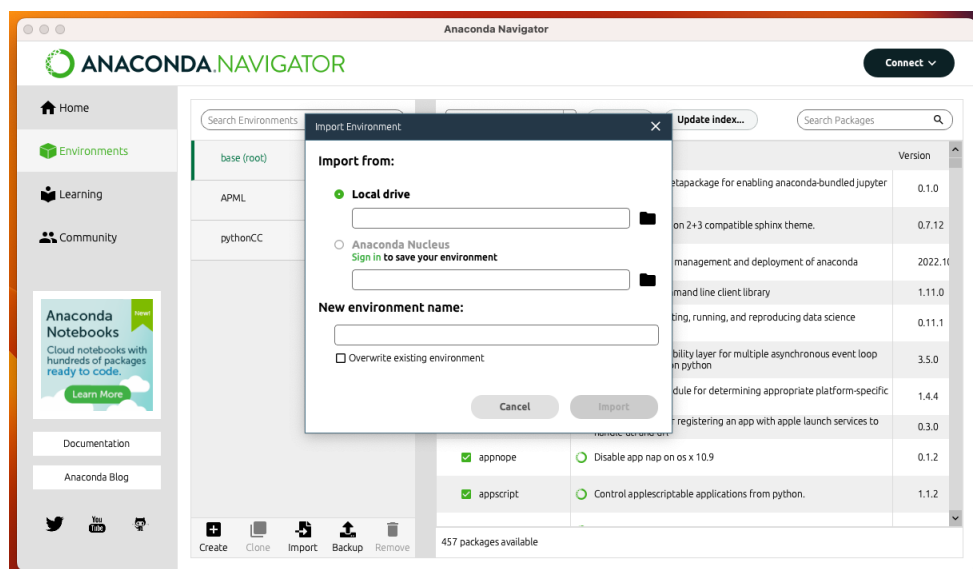


# Setting up an environment with Anaconda Navigator

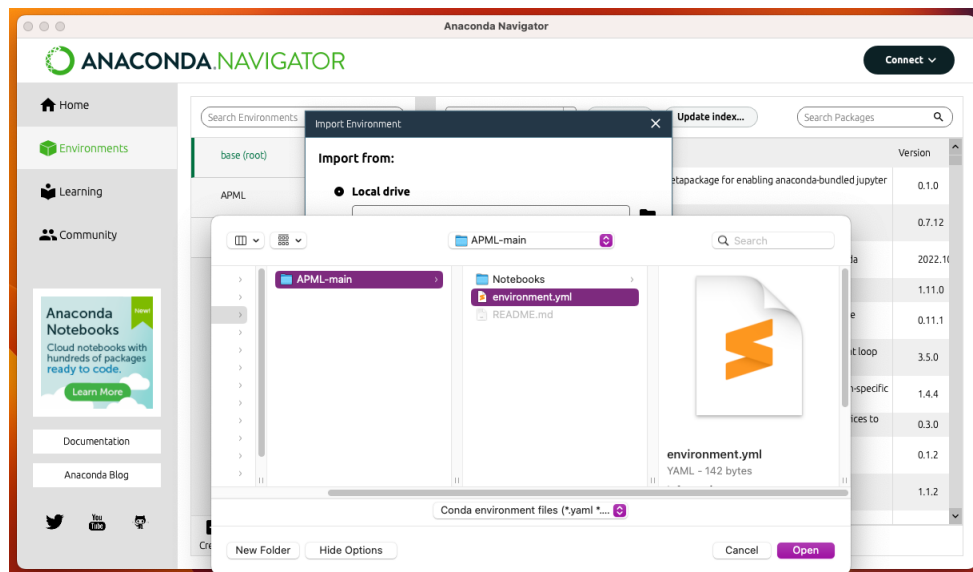
**Step 1:** Open Anaconda Navigator. Go to “**Environments**” in the menu on the left and select “**Import**” in the bottom panel.



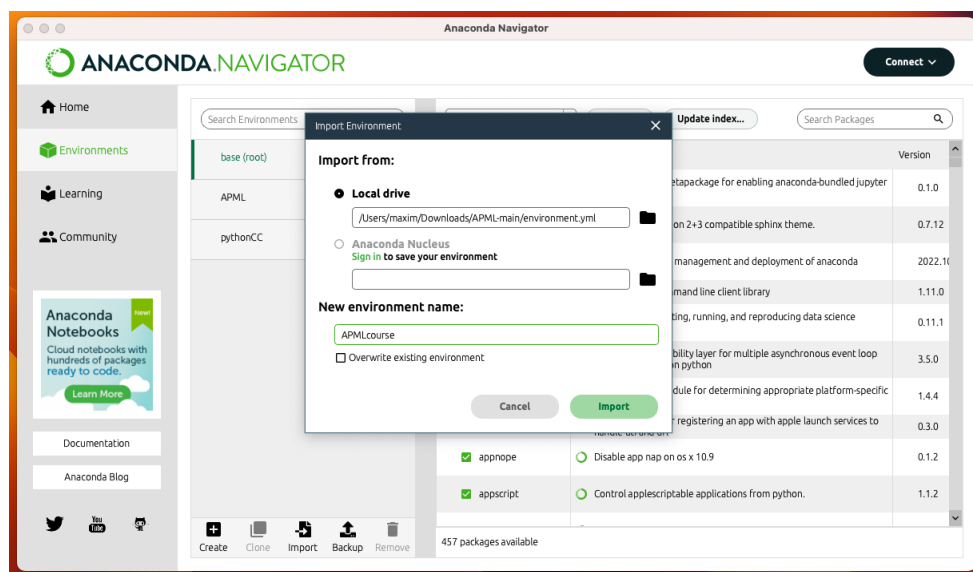
**Step 2:** Choose to import from “**Local drive**”.



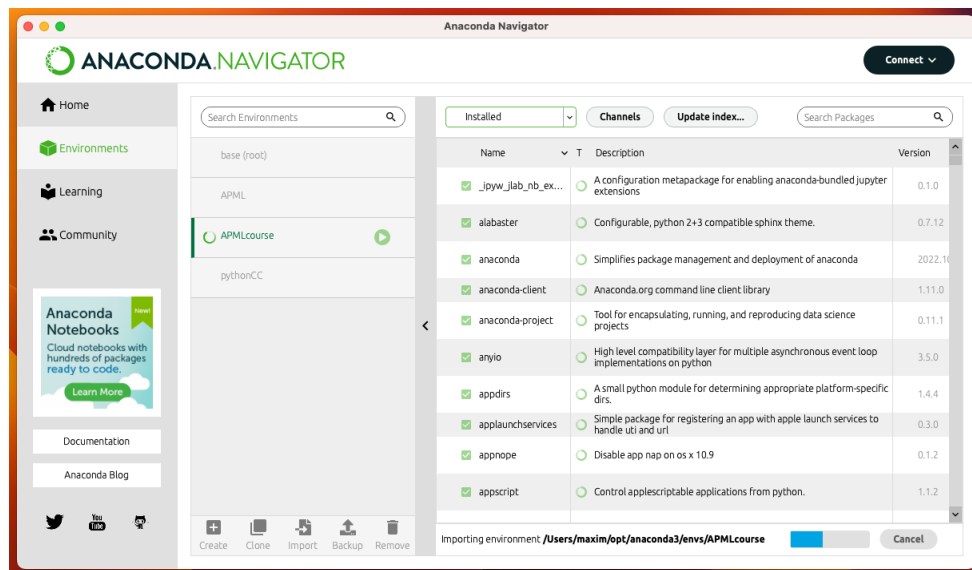
**Step 3:** Navigate to your local copy of the course material and select the “**environment.yml**” file we shared with you.



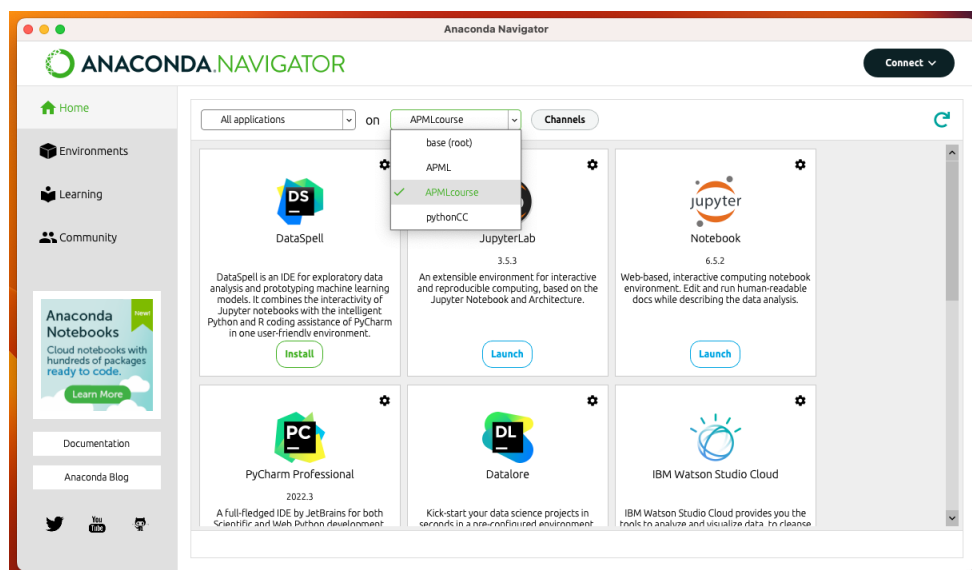
**Step 4:** Click “Import”.



**Step 5:** The environment packages will be installed (with a blue progress bar in the bottom right). This can take a few minutes.

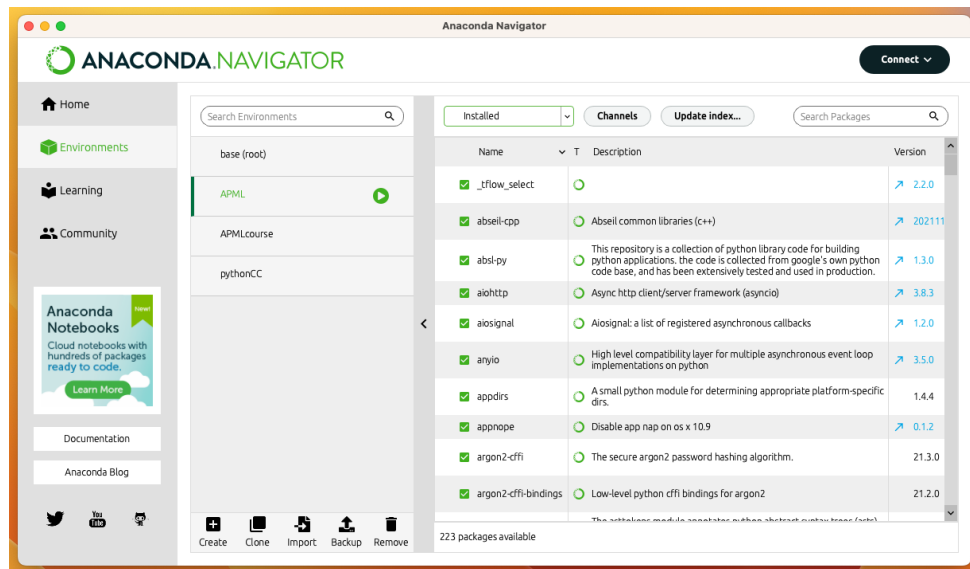


**Step 6:** As soon as the environment is set up, you can navigate back to “Home” in the menu on the left. Make sure you select the installed environment. Now you can start JupyterLab and all required packages are ready!

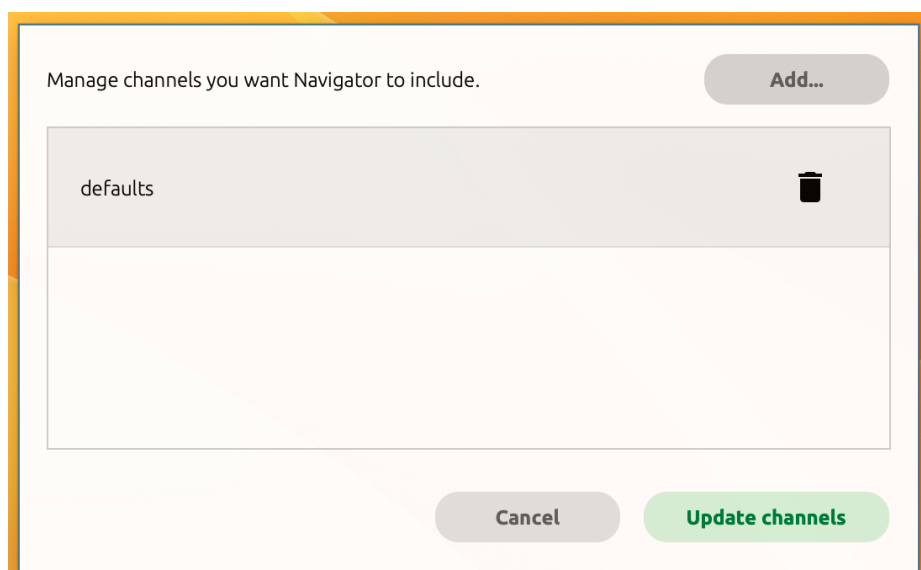


# Add a package to an environment with Anaconda Navigator

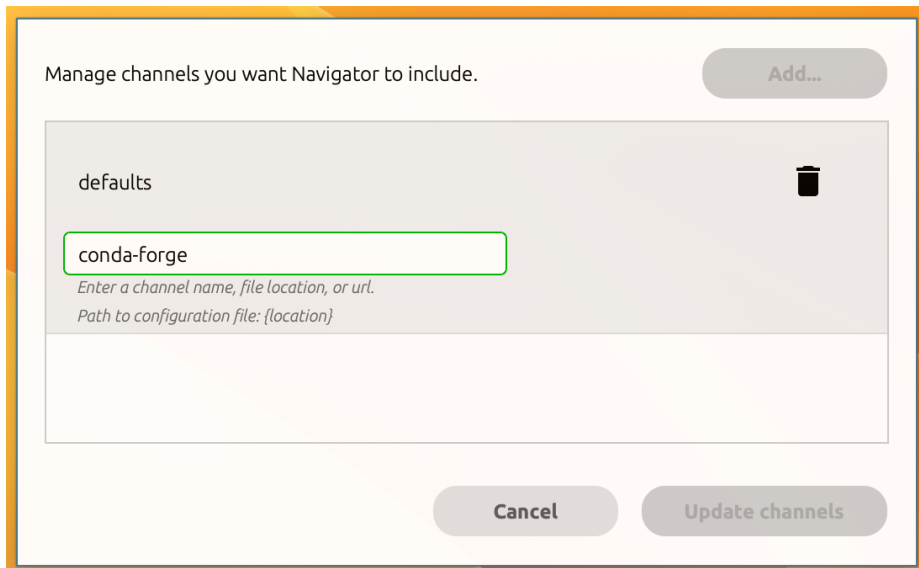
**Step 1:** Open Anaconda Navigator. Go to “**Environments**” in the menu on the left and select the environment in which you want to install the package, e.g. “**APML**”.




**Step 2:** Click on the “**Channels**” button. A new window pops up. Click on button “**Add**”.



**Step 3:** Add “conda-forge” as a new channel and click enter.

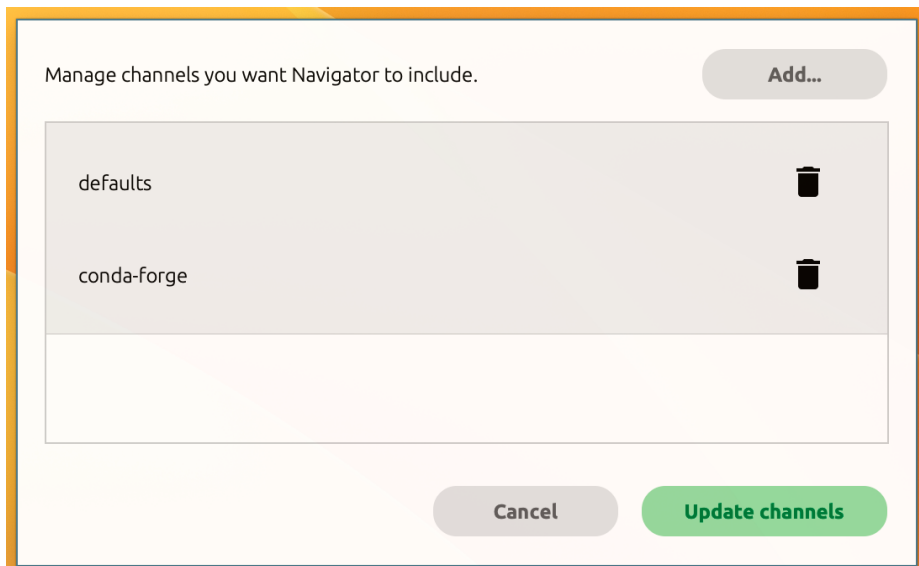


Manage channels you want Navigator to include. Add...



defaults	
<input type="text" value="conda-forge"/>	
<small>Enter a channel name, file location, or url. Path to configuration file: {location}</small>	

Cancel Update channels

**Step 4:** When the new channel is added, click the “Update channels” button.

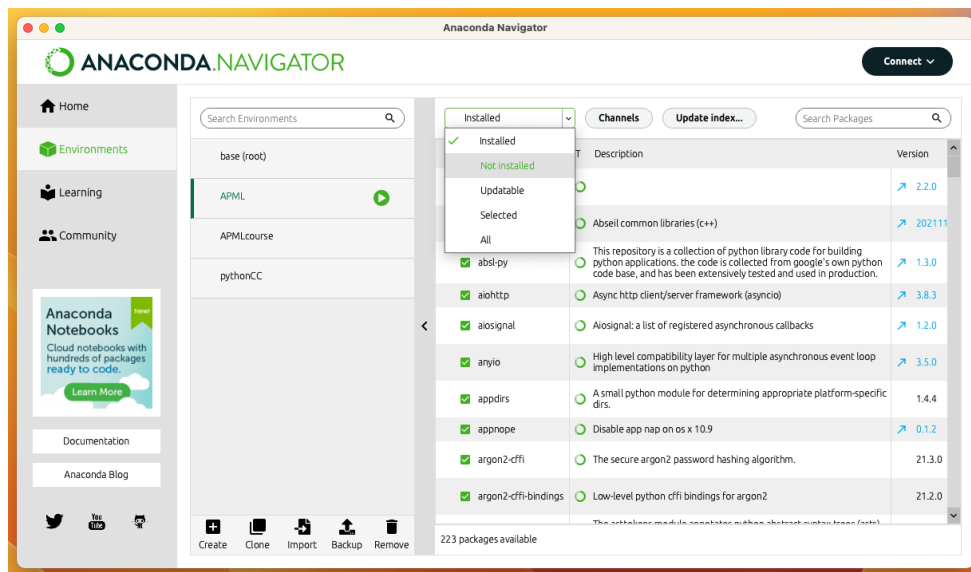


Manage channels you want Navigator to include. Add...

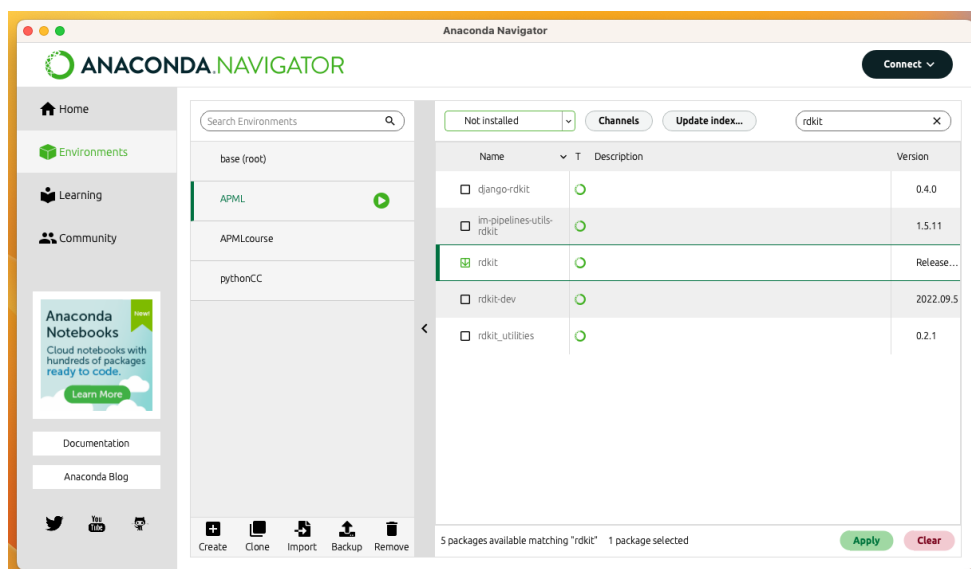
defaults	
conda-forge	

Cancel Update channels

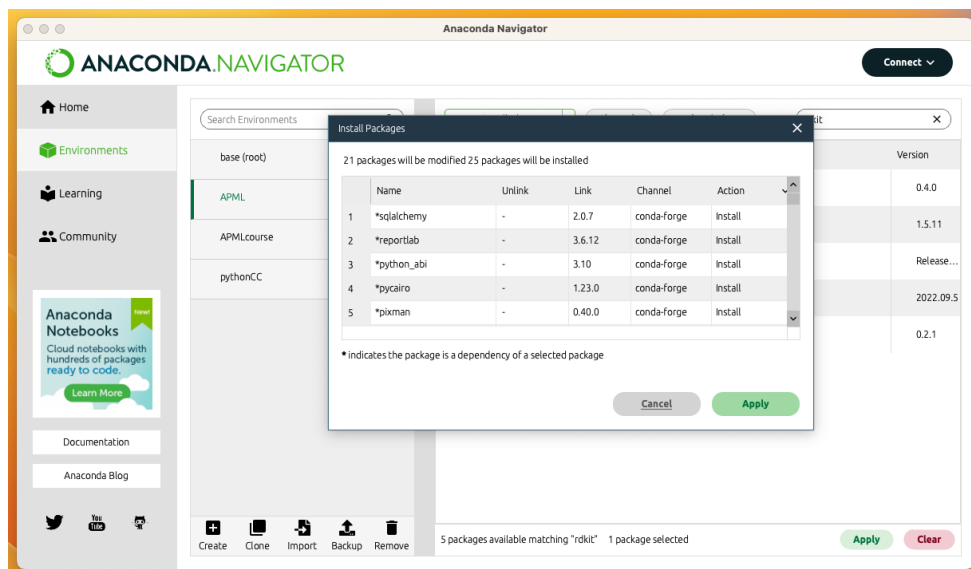
**Step 5:** Choose “Not installed” in the drop-down menu.



**Step 6:** In the top-right corner you can put in “Search Packages” field the package you want to install, e.g. “rdkit” or “deepsmls”. Select the respective package and click the “Apply” button.



**Step 7:** The required (additional) packages will be searched. Note that this can take several minutes or longer. When all required packages are found, click **“Apply”** to install the package. Note that this can again take several minutes to half an hour.



**Step 8:** As soon you have installed all packages, you can return to **“Home”**. Make sure that the correct environment **“APML”** is selected and start **“JupyterLab”**.

