APEX Tutorial

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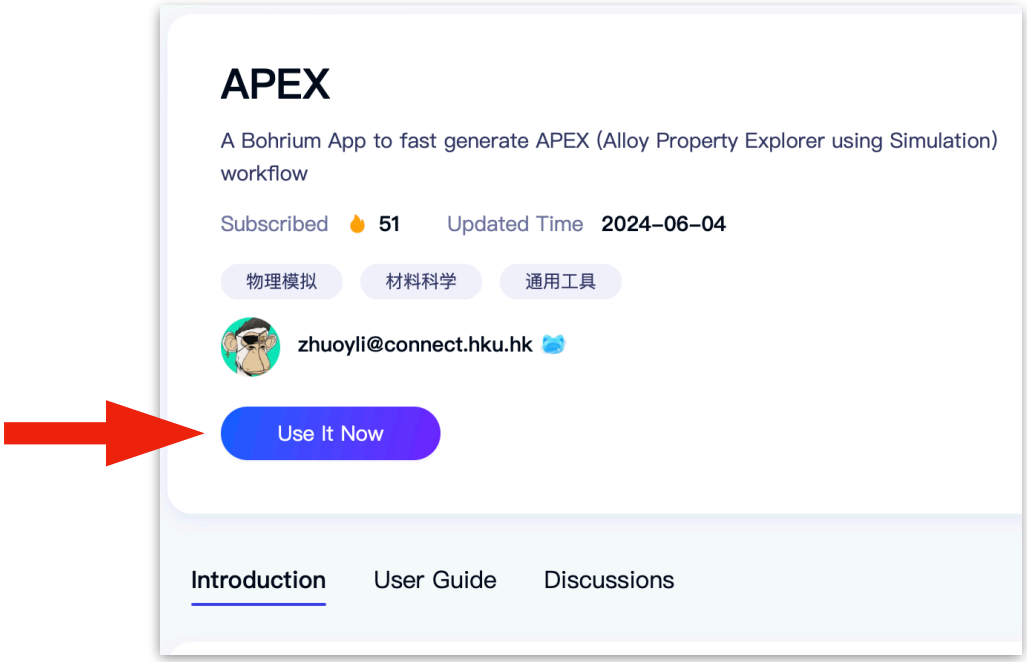
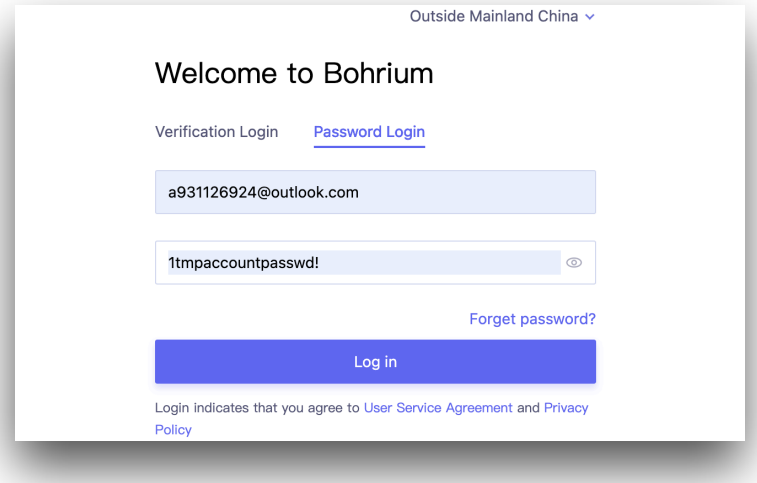
A. Hands-on APEX Bohrium App

Here we demonstrate how to use APEX Bohrium APP by submitting a computational workflow with the **EAM** pair potential using **LAMMPS** to calculate the **EOS curve** and **elastic properties** of **titanium**.

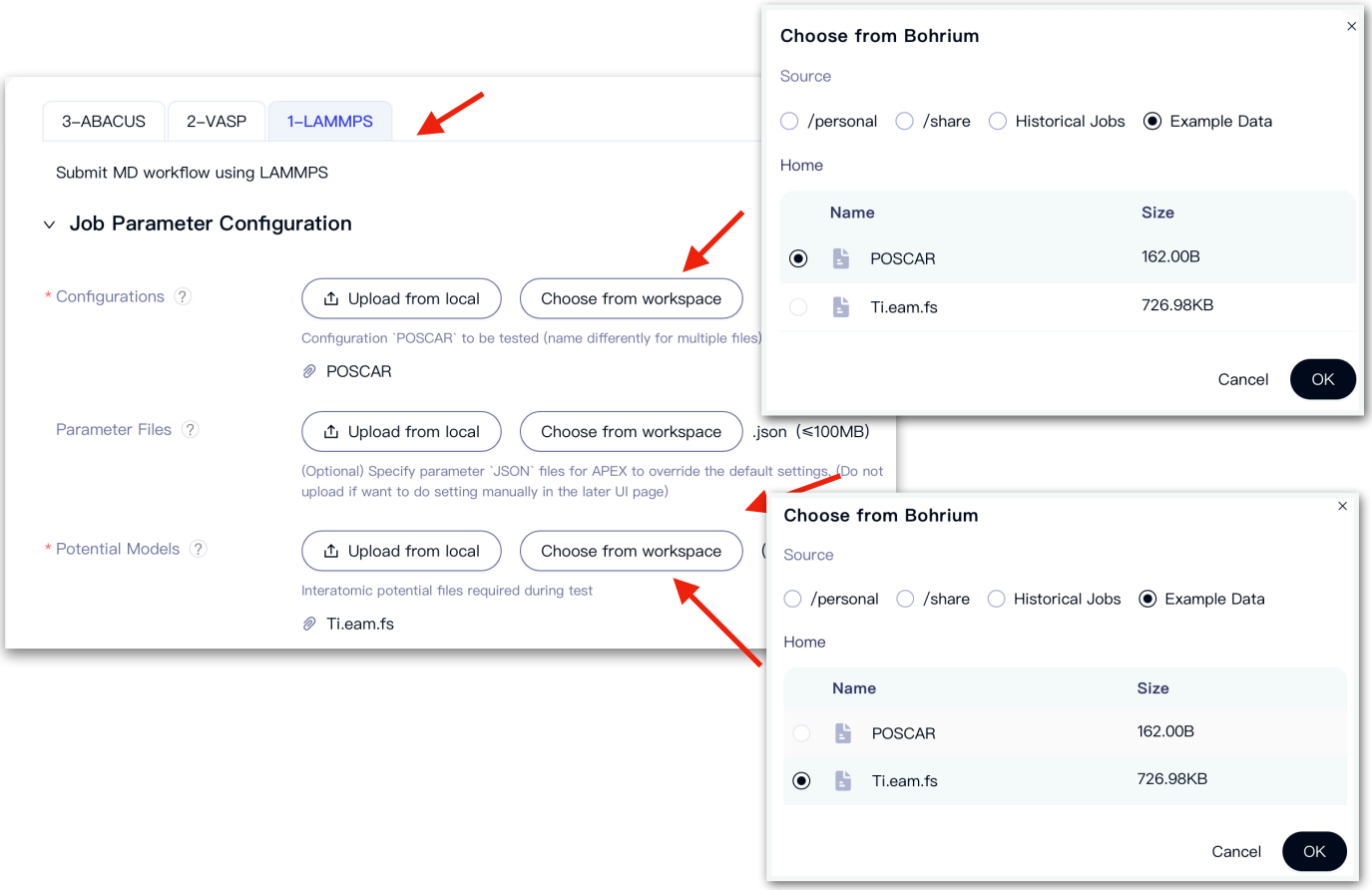
1. Click here to enter the main page of **APEX Bohrium App** (https://bohrium.dp.tech/apps/apex?tab=readme_link), Click the **Use It Now** Button and use following pre-registered temporary Bohrium account to login:

   Email: a931126924@outlook.com
   Password: 1tmpaccountpasswd!

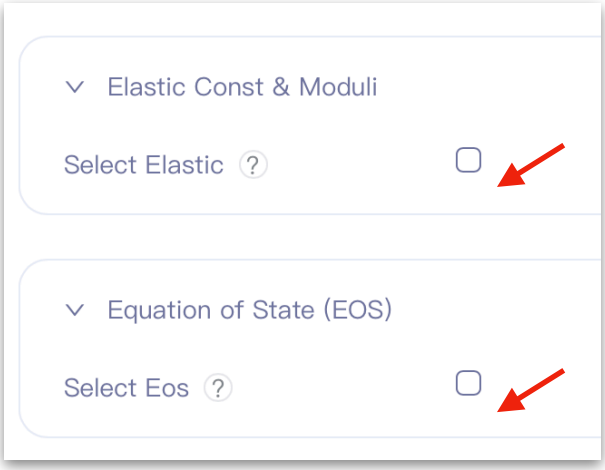




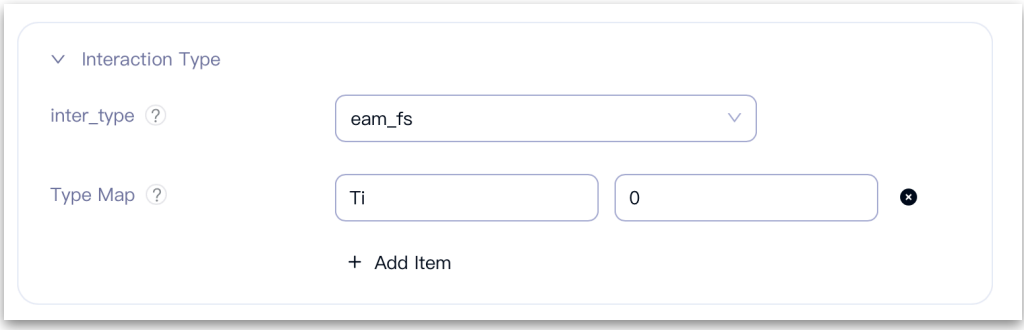
2. In the **Form** page, choose **'1–LAMMPS'** on the top of the parameter page. Drop the page down, and choose two example files from **'Example Data'** accordingly:



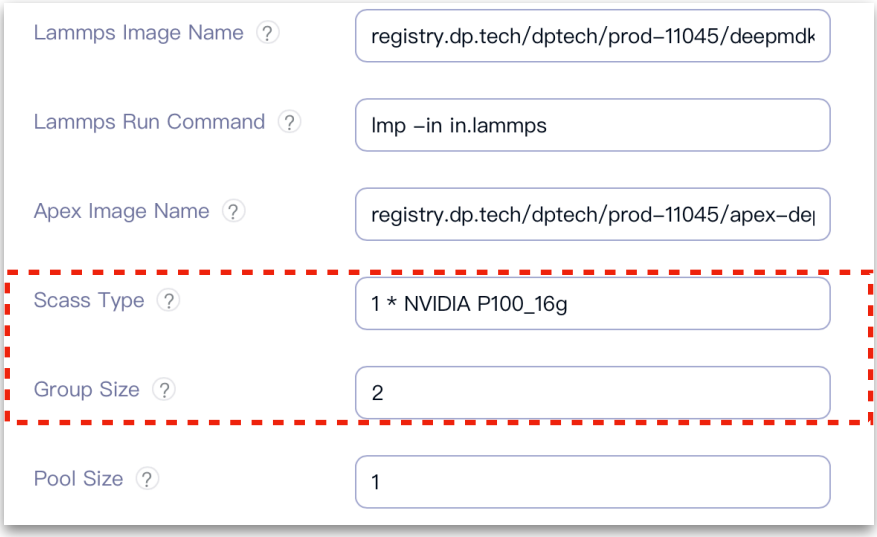
3. Next, drop down the page and check **"Select Elastic"** and **"Select Eos"** in the series of property type boxes. Upon selection, the configuration for computational parameters will expand.



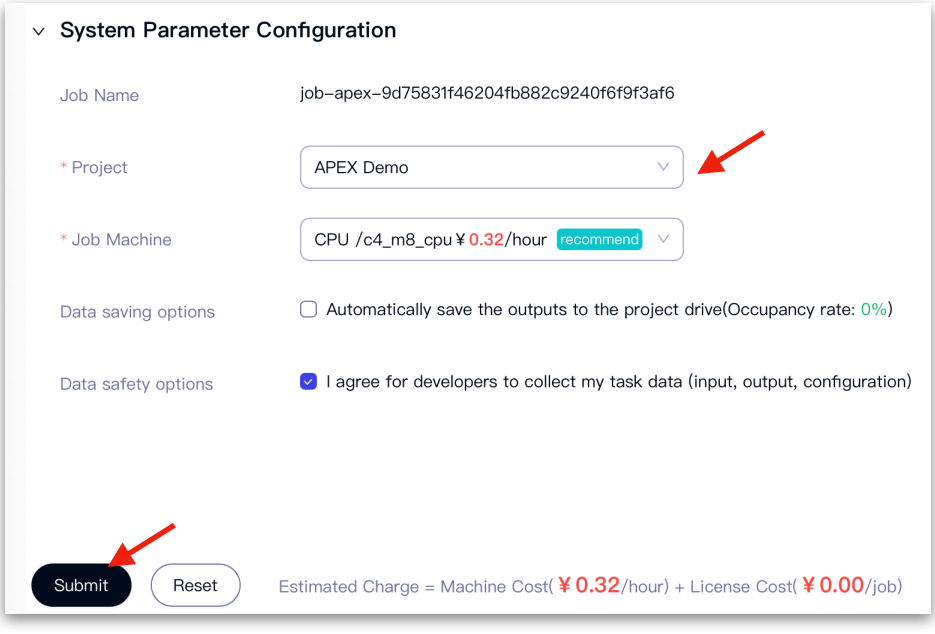
4. Down to the **“Interaction Type”** sub-region, Set up atomic interaction details. Select **"eam_fs"** from the **Inter Type** dropdown, and add **Ti: 0** in the **Type Map** area.



5. Below the **“Interaction Type”** sub-region, change the **“Scass Type”** to **1 * NVIDIA P100_16g** for faster resource scheduling, and then change **“Group Size”** to **2**

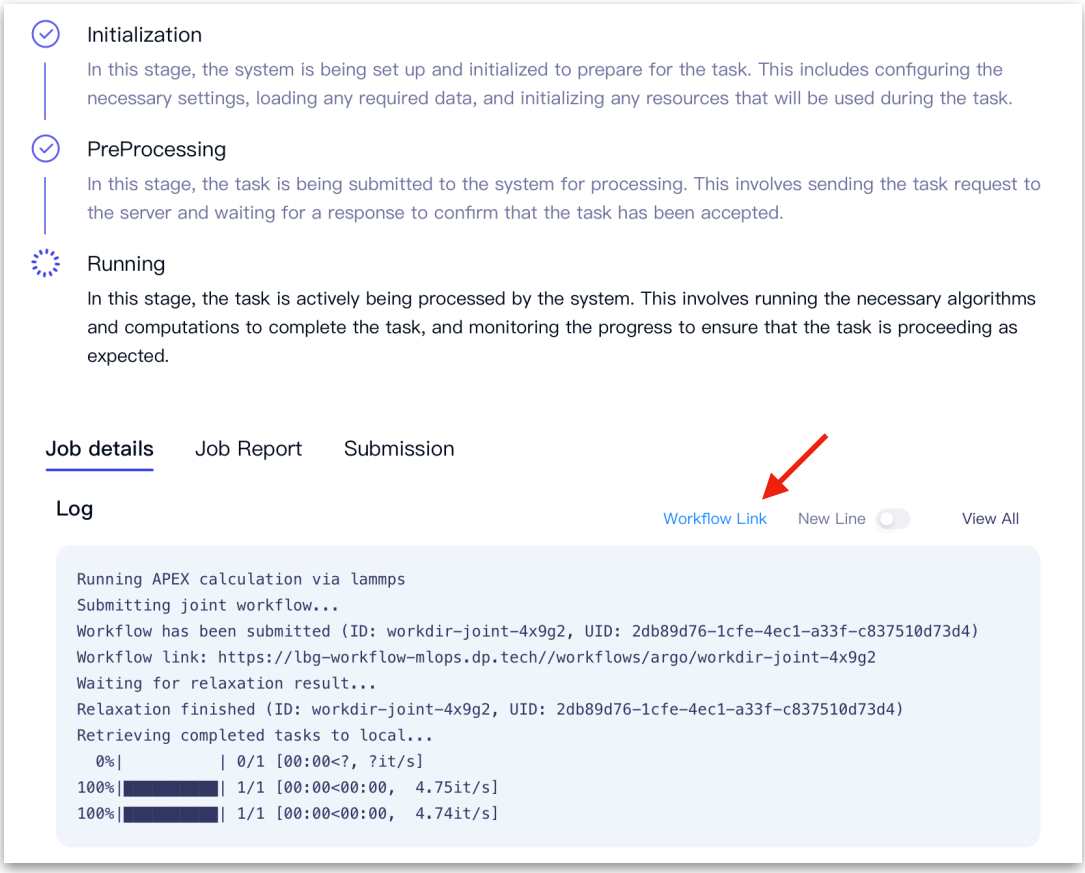


6. Drop to the bottom at **“System Parameter Configuration”** sub-section, Select **‘APEX Demo’ or your own project** in **Project** dropdown, then click the **Submit** button

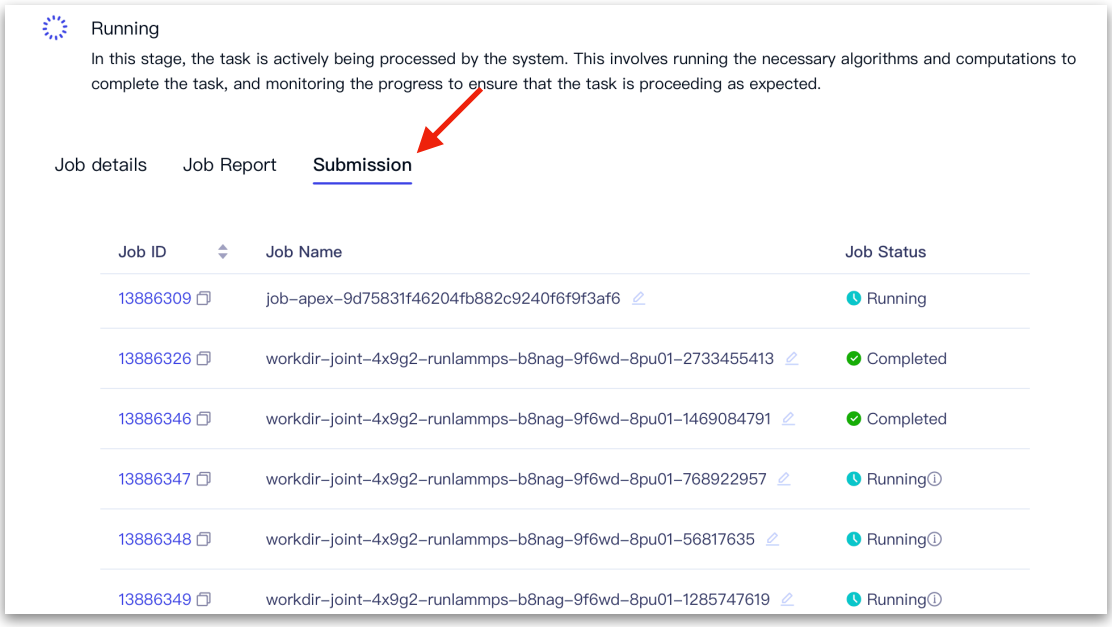


7. Next, click ‘**Job details**’ for workflow monitoring page

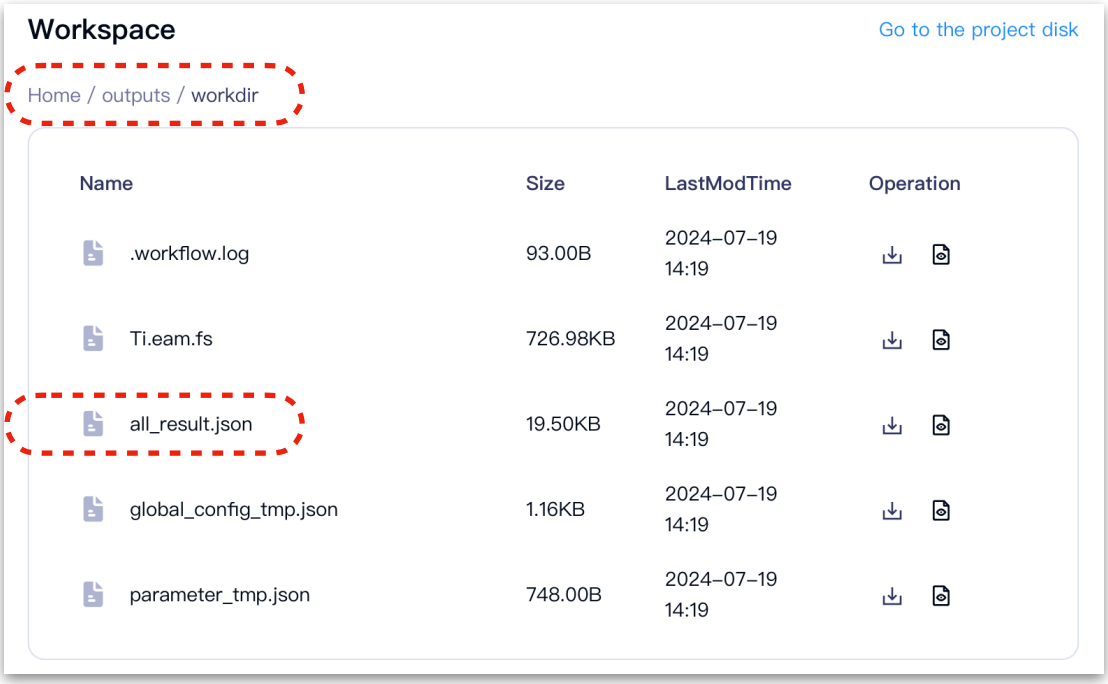
8. On this page, you can monitor the progress of tasks. When the **“Workflow Link"** appears at the right, you can click it to access the Argo workflow monitoring UI page.



9. You can also click the **“submission"** tab to see detailed running status of all submitted tasks:



10. Upon completion of the calculations, all working directories and result files are automatically collected in the /outputs/workdir/ directory, where users can browse and download them into local. The **'all_result.json'** file can be visualized by `apex report –w all_result.json` command of any APEX pre–installed GUI computer.

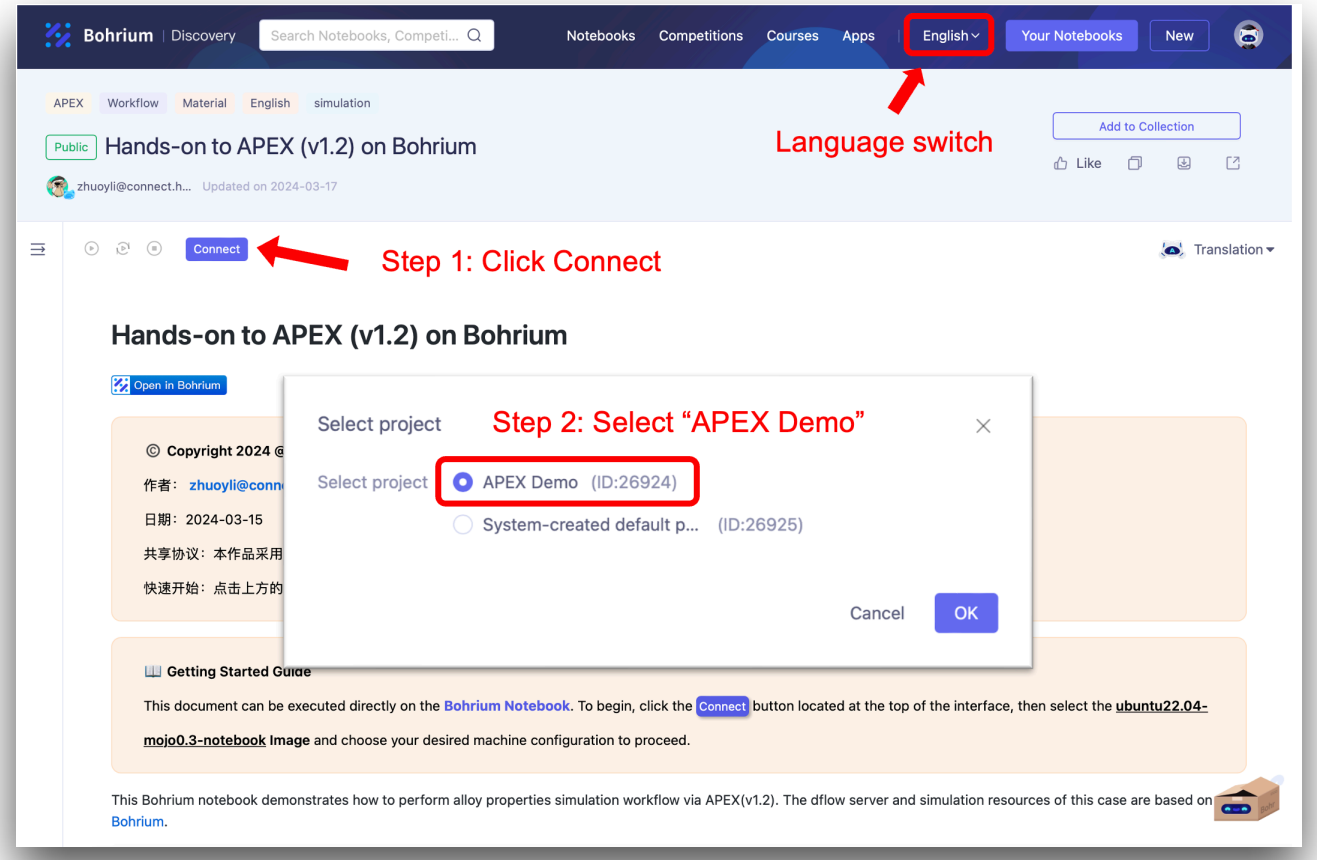


B. Hands–on terminal submission on Bohrium

Please use the following pre–registered temporary Bohrium platform account to access the **hands–on demonstration example notebook** of APEX

Email: a931126924@outlook.com
Password: 1tmpaccountpasswd!
Project_id: 26924

Tutorial Notebook link: https://nb.bohrium.dp.tech/detail/26383176824


Bohrium | Discovery
Search Notebooks, Competi...
Notebooks
Competitions
Courses
Apps
English
Your Notebooks
New
APEX
Workflow
Material
English
simulation
Public
Hands-on to APEX (v1.2) on Bohrium
zhuoyli@connect.h...
Updated on 2024-03-17
Language switch
Add to Collection
Like
Connect
Step 1: Click Connect
Translation
Hands-on to APEX (v1.2) on Bohrium
Open in Bohrium
Select project
Step 2: Select “APEX Demo”
Select project
APEX Demo (ID:26924)
System-created default p... (ID:26925)
Cancel
OK
© Copyright 2024 @
作者： zhuoyli@conn
日期：2024-03-15
共享协议：本作品采用
快速开始：点击上方的
Getting Started Guide
This document can be executed directly on the Bohrium Notebook. To begin, click the Connect button located at the top of the interface, then select the ubuntu22.04-mojo0.3-notebook Image and choose your desired machine configuration to proceed.
This Bohrium notebook demonstrates how to perform alloy properties simulation workflow via APEX(v1.2). The dflow server and simulation resources of this case are based on Bohrium.