APEX Tutorial

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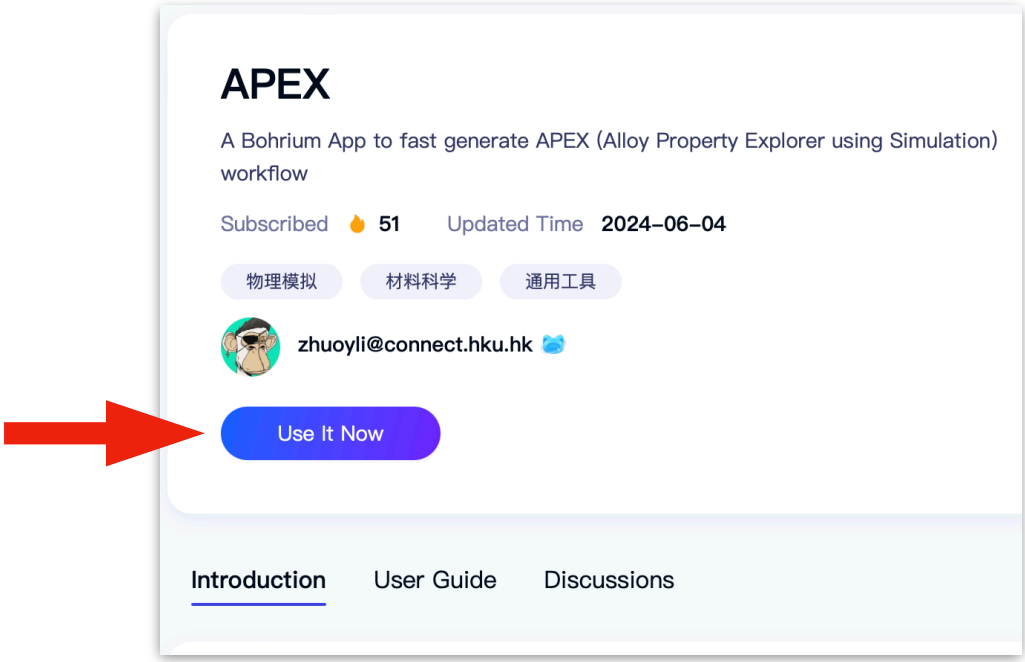
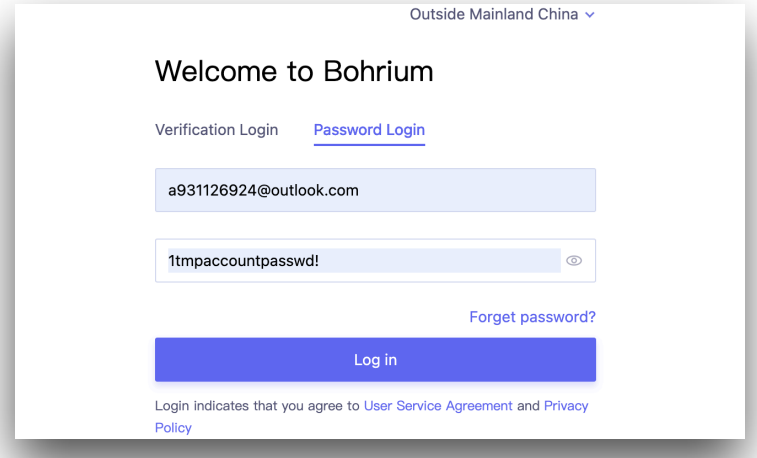
A. Hands-on APEX Bohrium App

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**.

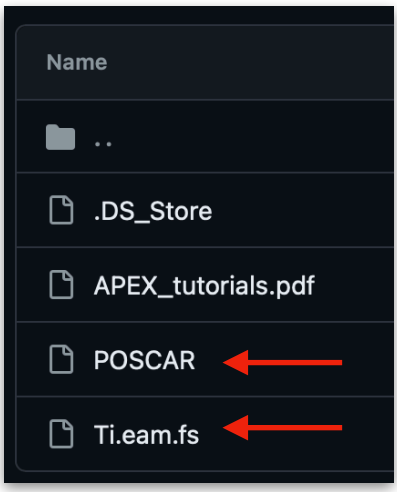
1. Click here to enter the main page of **APEX Bohrium App** (https://bohrium.dp.tech/apps/apex?tab=readme_link), Click the **Use It Now** Button and use following pre-registered temporary Bohrium account to login:

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

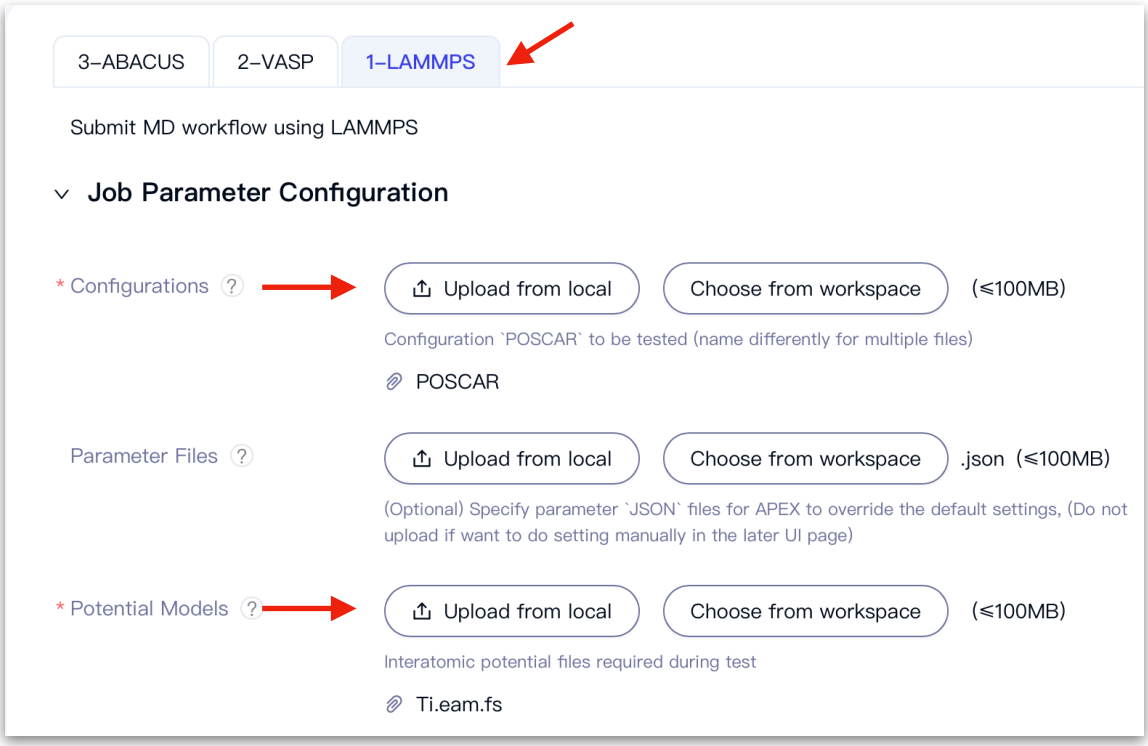




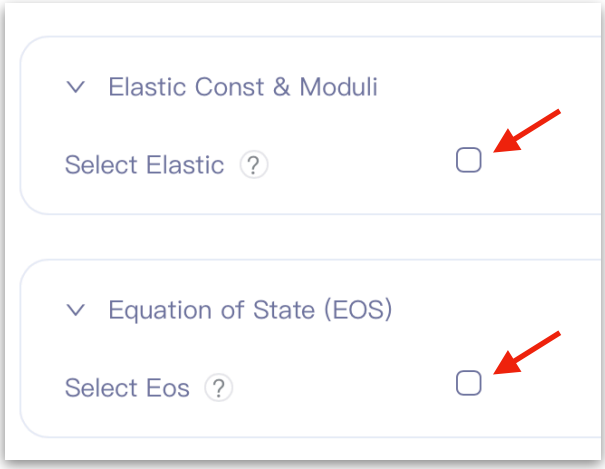
2. Download two files: the **POSCAR** of HCP Ti (POSCAR.Ti.hcp) and **EAM potential** file of Ti (Ti.eam.fs) from https://github.com/ZLI-afk/static/tree/main/docs/apex_Ti_test/tutorial



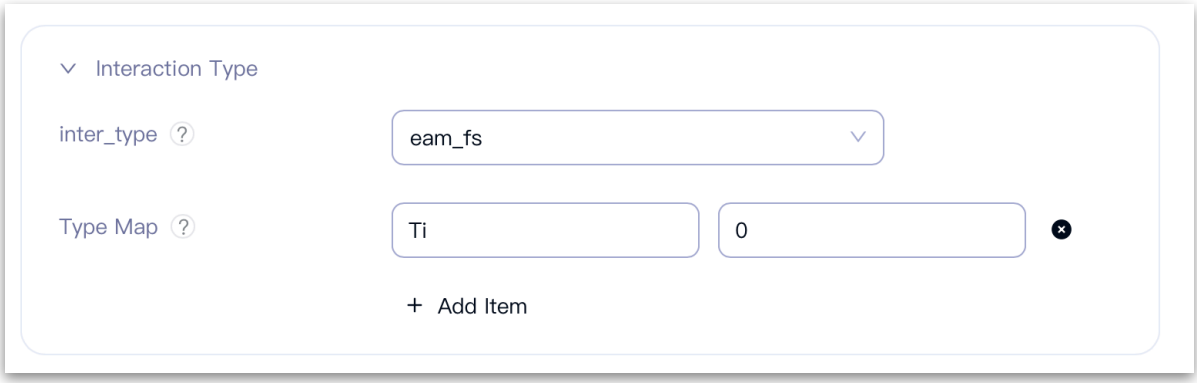
3. Return to the **Form** page, then choose **'1-LAMMPS'** on the top of the parameter page. Drop the page down, and upload above two files accordingly:



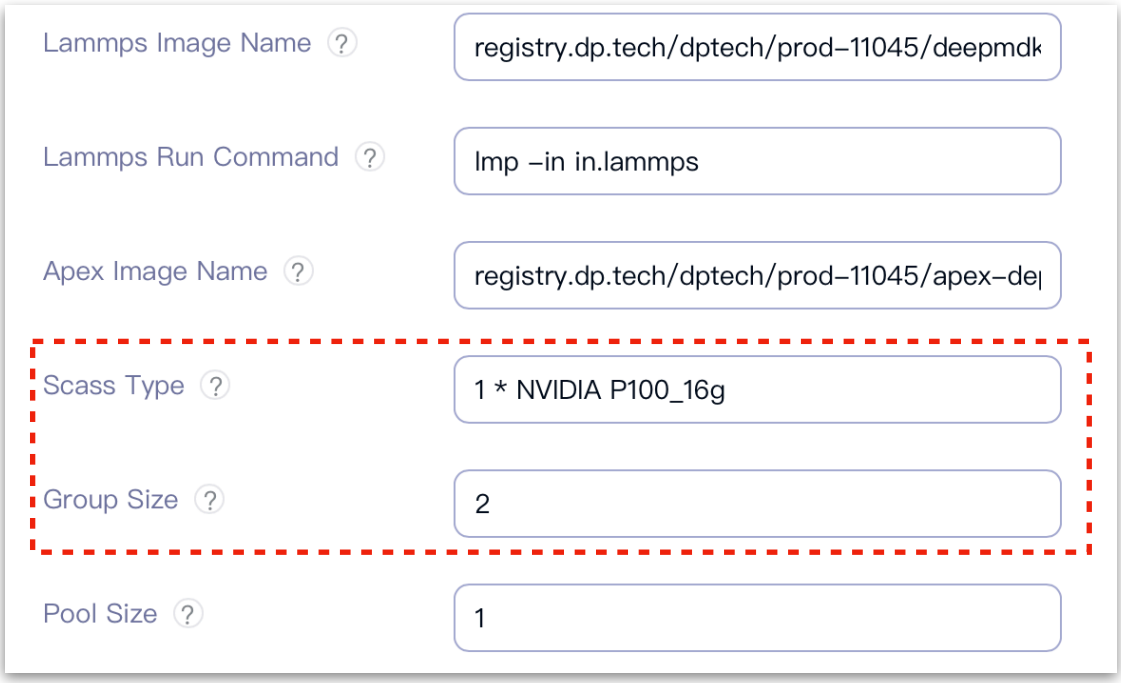
4. Next, drop down the page and check **"Select Elastic"** and **"Select Eos"** in the series of property type boxes. Upon selection, the configuration for computational parameters will expand.



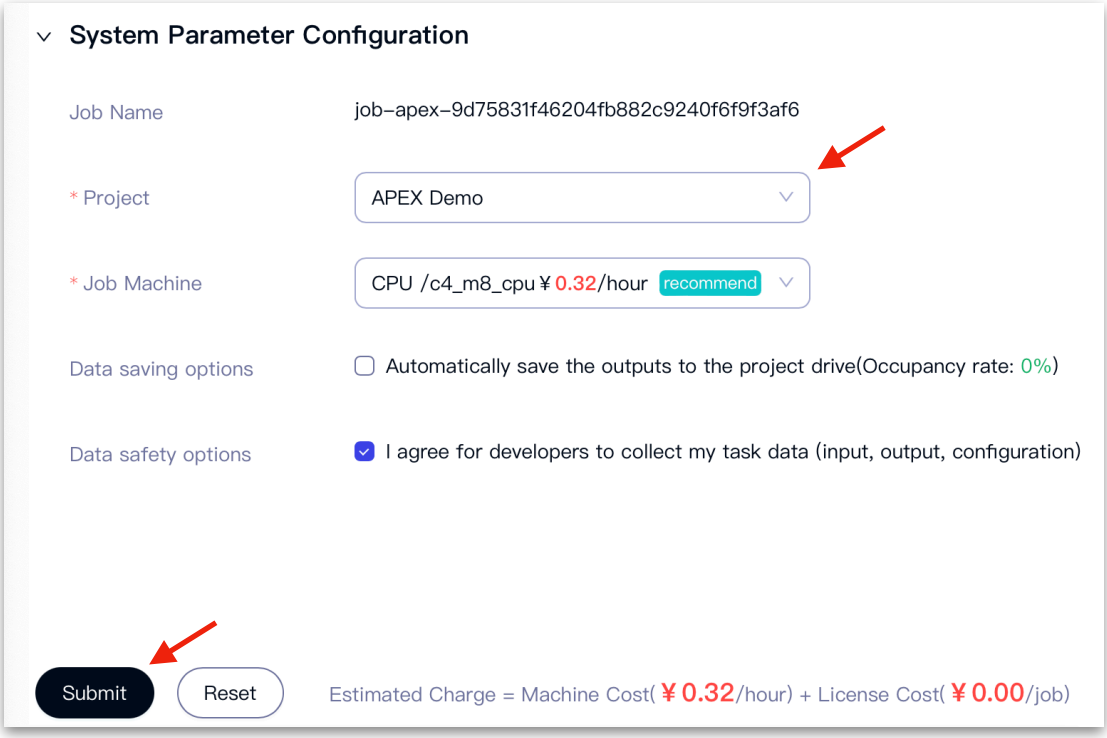
5. Down to the **“Interaction Type”** sub–region, Set up atomic interaction details. Select **"eam_fs"** from the **Inter Type** dropdown, and add **Ti: 0** in the **Type Map** area.



6. 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**

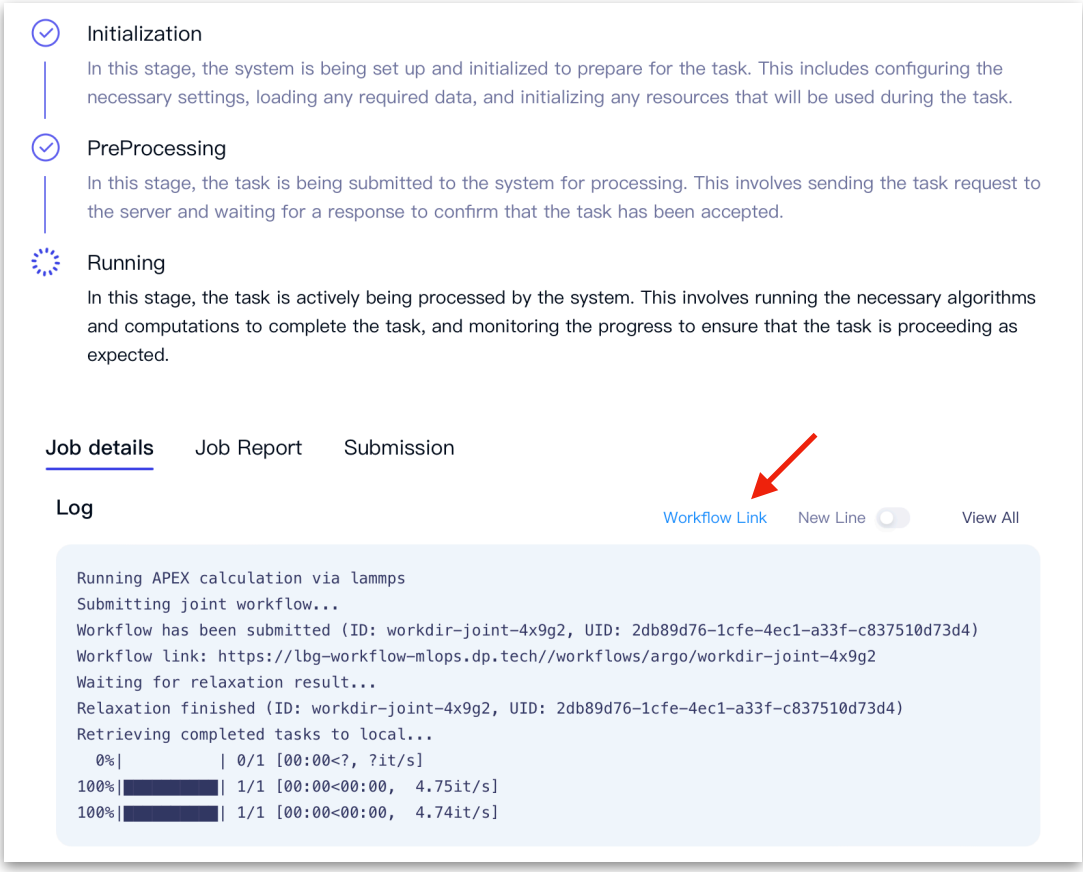


7. Drop to the bottom at **“System Parameter Configuration”** sub-section, Select **‘APEX Demo’** in **Project** dropdown, then click the **Submit** button

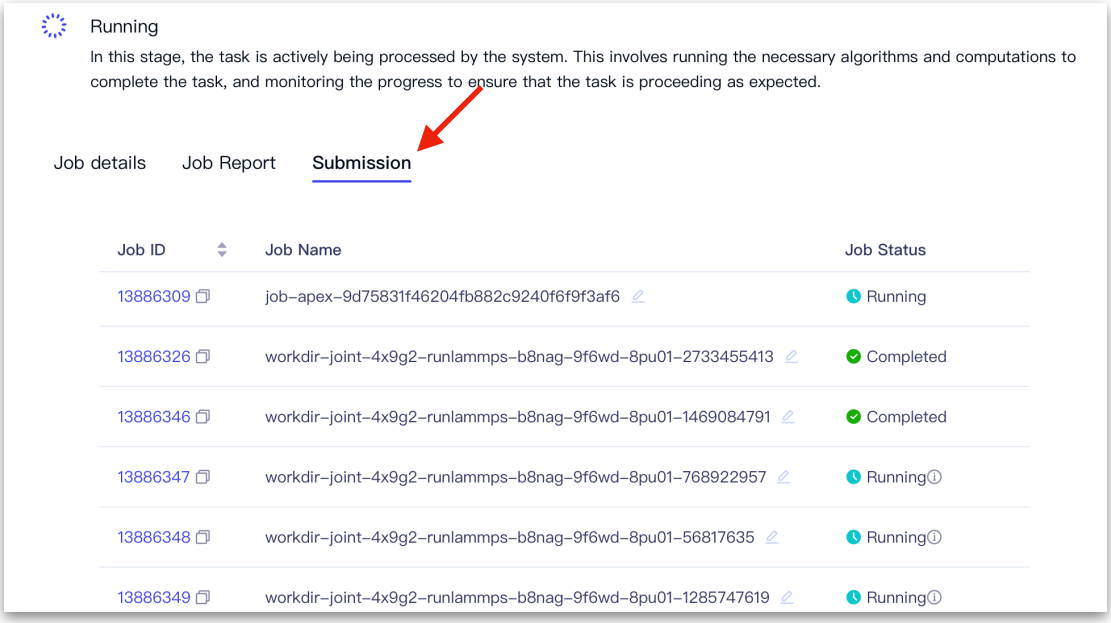


8. Next, click **‘Job details’** for workflow monitoring page

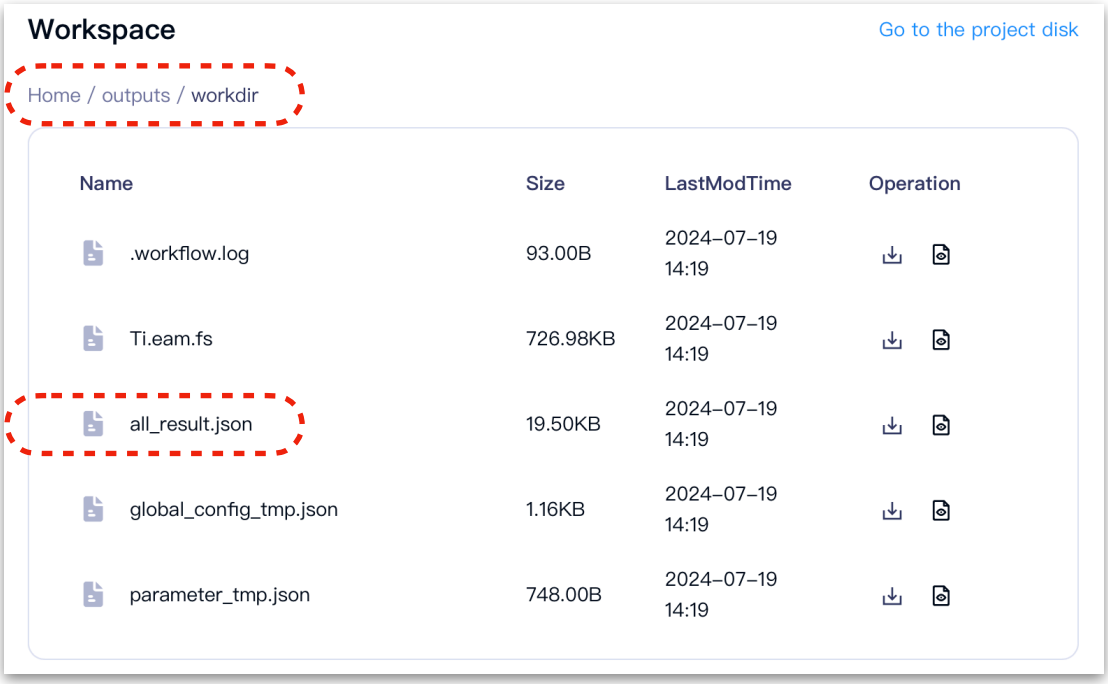
9. On this page, you can monitor the progress of tasks. When the **“Workflow Link"** appears at the right, you can click it to access the Argo workflow monitoring UI page.



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



11. 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