

APEX Tutorial

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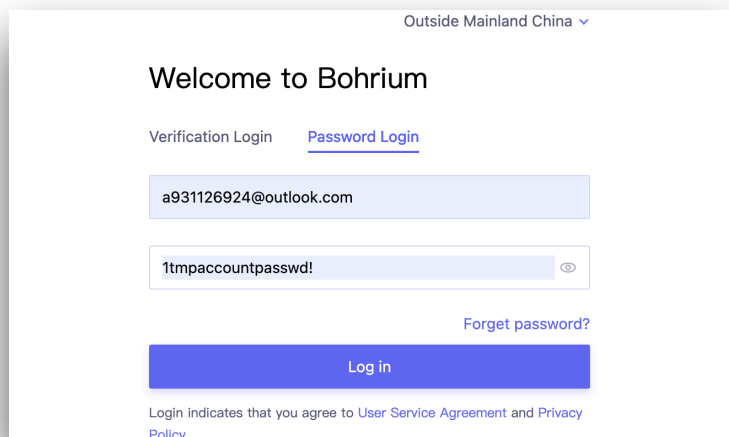
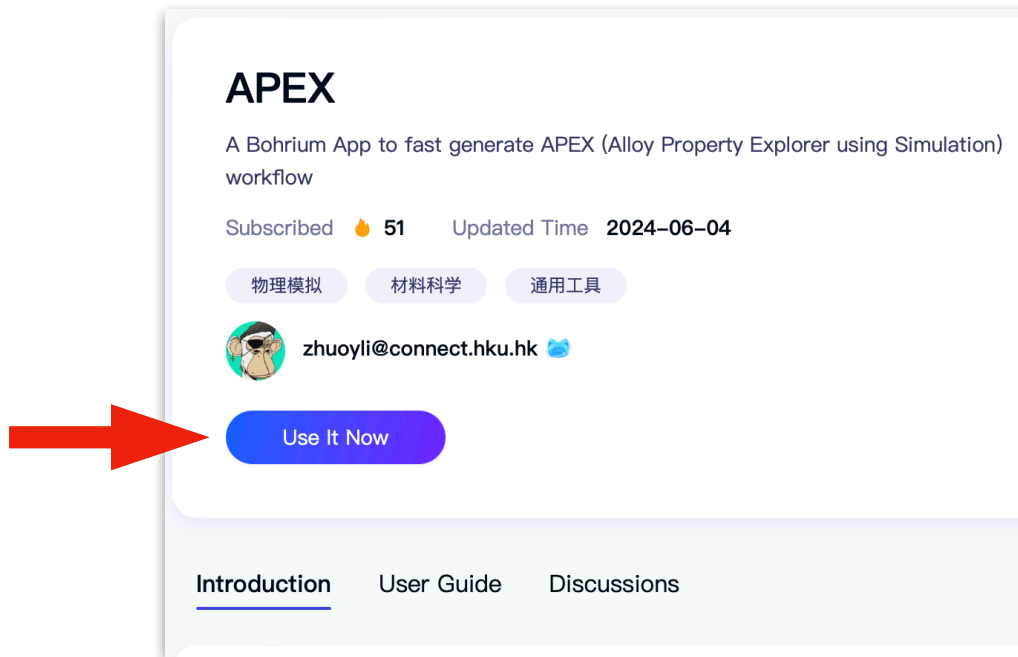
A. Hands-on APEX Bohrium App

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](https://bohrium.dp.tech/apps/apex?tab=readme_link) 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:

The screenshot shows the '1-LAMMPS' configuration page. At the top, there are tabs for '3-ABACUS', '2-VASP', and '1-LAMMPS'. Below the tabs, the text 'Submit MD workflow using LAMMPS' is displayed. The 'Job Parameter Configuration' section is expanded, showing three categories: 'Configurations', 'Parameter Files', and 'Potential Models'. Each category has 'Upload from local' and 'Choose from workspace' buttons. Two 'Choose from Bohrium' modal windows are open. The first modal is for the 'Configurations' category, showing a table with two files: 'POSCAR' (162.00B) and 'Ti.eam.fs' (726.98KB). The second modal is for the 'Parameter Files' category, showing the same two files. Red arrows point to the '1-LAMMPS' tab, the 'Choose from workspace' button for 'Configurations', and the 'Choose from workspace' button for 'Parameter Files'.

3-ABACUS 2-VASP 1-LAMMPS

Submit MD workflow using LAMMPS

Job Parameter Configuration

* Configurations ?

Upload from local Choose from workspace

Configuration 'POSCAR' to be tested (name differently for multiple files)

POSCAR

Parameter Files ?

Upload from local Choose from workspace .json (≤100MB)

(Optional) Specify parameter 'JSON' files for APEX to override the default settings. (Do not upload if want to do setting manually in the later UI page)

* Potential Models ?

Upload from local Choose from workspace

Interatomic potential files required during test

Ti.eam.fs

Choose from Bohrium

Source

☐ /personal ☐ /share ☐ Historical Jobs ☒ Example Data

Home

Name	Size
<input checked="" type="radio"/> POSCAR	162.00B
<input type="radio"/> Ti.eam.fs	726.98KB

Cancel OK

Choose from Bohrium

Source

☐ /personal ☐ /share ☐ Historical Jobs ☒ Example Data

Home

Name	Size
<input type="radio"/> POSCAR	162.00B
<input checked="" type="radio"/> Ti.eam.fs	726.98KB

Cancel OK

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.

The screenshot shows two sections of the configuration page. The first section is 'Elastic Const & Moduli' with a 'Select Elastic ?' checkbox. The second section is 'Equation of State (EOS)' with a 'Select Eos ?' checkbox. Red arrows point to the 'Select Elastic ?' and 'Select Eos ?' checkboxes.

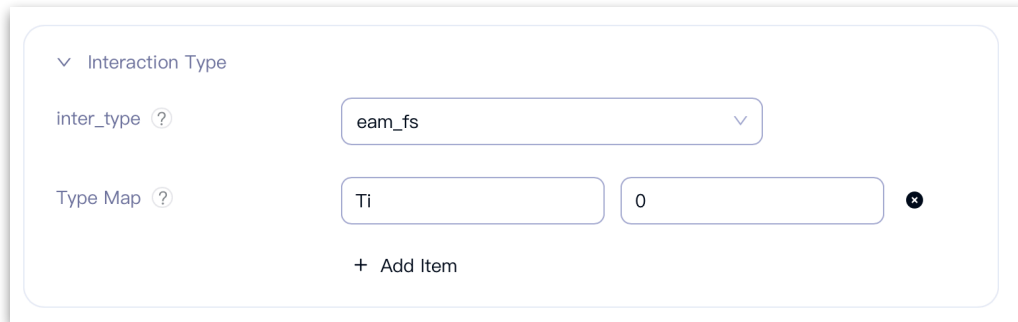
Elastic Const & Moduli

Select Elastic ?

Equation of State (EOS)

Select Eos ?

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.



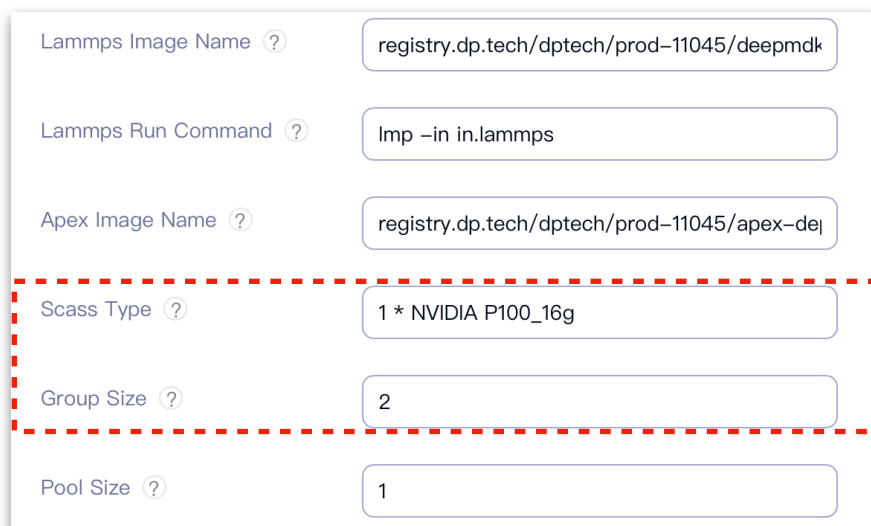
Interaction Type

Inter_type ? eam_fs

Type Map ? Ti 0 *

+ Add Item

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**



Lammps Image Name ? registry.dp.tech/dptech/prod-11045/deepmdk

Lammps Run Command ? Imp -in in.lammps

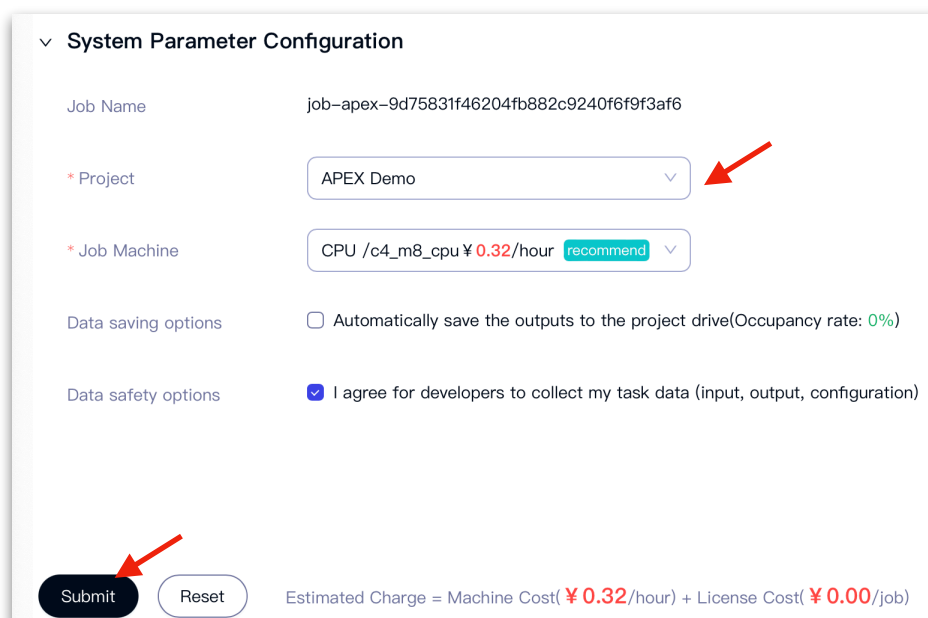
Apex Image Name ? registry.dp.tech/dptech/prod-11045/apex-dei

Scass Type ? 1 * NVIDIA P100_16g

Group Size ? 2

Pool Size ? 1

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



System Parameter Configuration

Job Name job-apex-9d75831f46204fb882c9240f6f9f3af6

* Project APEX Demo

* Job Machine CPU /c4_m8_cpu ¥ 0.32/hour recommend

Data saving options ☐ Automatically save the outputs to the project drive(Occupancy rate: 0%)

Data safety options ☒ I agree for developers to collect my task data (input, output, configuration)

Submit Reset

Estimated Charge = Machine Cost(¥ 0.32/hour) + License Cost(¥ 0.00/job)

- Next, click **'Job details'** for workflow monitoring page
- 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.

The screenshot shows the 'Job details' page with three stages: Initialization, PreProcessing, and Running. The 'Running' stage is active. Below the stages, there are tabs for 'Job details', 'Job Report', and 'Submission'. The 'Log' section displays the workflow progress, including the submission of a joint workflow and the retrieval of completed tasks. A red arrow points to the 'Workflow Link' text in the log.

Initialization
In this stage, the system is being set up and initialized to prepare for the task. This includes configuring the necessary settings, loading any required data, and initializing any resources that will be used during the task.

PreProcessing
In this stage, the task is being submitted to the system for processing. This involves sending the task request to the server and waiting for a response to confirm that the task has been accepted.

Running
In this stage, the task is actively being processed by the system. This involves running the necessary algorithms and computations to complete the task, and monitoring the progress to ensure that the task is proceeding as expected.

Job details Job Report Submission

Log [Workflow Link](#) New Line View All

```
Running APEX calculation via lammmps
Submitting joint workflow...
Workflow has been submitted (ID: workdir-joint-4x9g2, UID: 2db89d76-1cfe-4ec1-a33f-c837510d73d4)
Workflow link: https://lbg-workflow-mlops.dp.tech/workflows/argo/workdir-joint-4x9g2
Waiting for relaxation result...
Relaxation finished (ID: workdir-joint-4x9g2, UID: 2db89d76-1cfe-4ec1-a33f-c837510d73d4)
Retrieving completed tasks to local...
0%|          | 0/1 [00:00<?, ?it/s]
100%|███████| 1/1 [00:00<00:00, 4.75it/s]
100%|███████| 1/1 [00:00<00:00, 4.74it/s]
```

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

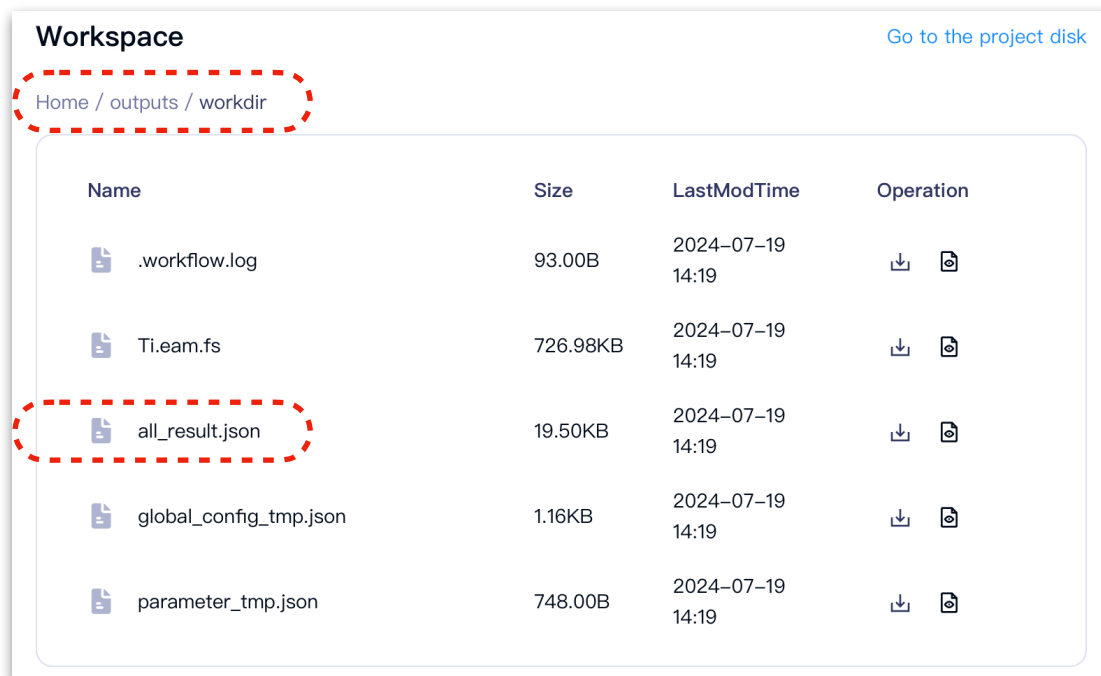
The screenshot shows the 'Submission' tab with a table of job details. A red arrow points to the 'Submission' tab. The table has columns for Job ID, Job Name, and Job Status.

Running
In this stage, the task is actively being processed by the system. This involves running the necessary algorithms and computations to complete the task, and monitoring the progress to ensure that the task is proceeding as expected.

Job details Job Report **Submission**

Job ID	Job Name	Job Status
13886309	job-apex-9d75831f46204fb882c9240f6f9f3af6	Running
13886326	workdir-joint-4x9g2-runlammmps-b8nag-9f6wd-8pu01-2733455413	Completed
13886346	workdir-joint-4x9g2-runlammmps-b8nag-9f6wd-8pu01-1469084791	Completed
13886347	workdir-joint-4x9g2-runlammmps-b8nag-9f6wd-8pu01-768922957	Running
13886348	workdir-joint-4x9g2-runlammmps-b8nag-9f6wd-8pu01-56817635	Running
13886349	workdir-joint-4x9g2-runlammmps-b8nag-9f6wd-8pu01-1285747619	Running

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>

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APEX Workflow Material English simulation

Public Hands-on to APEX (v1.2) on Bohrium

zhuoyli@connect.h... Updated on 2024-03-17

Add to Collection Like

Connect

Step 1: Click Connect

Hands-on to APEX (v1.2) on Bohrium

Open in Bohrium

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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-mojito0.3-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.

Select project Step 2: Select "APEX Demo"

Select project ☒ APEX Demo (ID:26924)

☐ System-created default p... (ID:26925)

Cancel OK