gsub (Open OnDemand)

Gaussian Job Submission

Gaussian job submission is performed in the following two steps:

1. **Data Preparation**: Set up the working directory and prepare input files
2. **Gaussian Settings**: Select/edit input, configure computational resources, and submit the job

You can switch between these steps using the tabs at the top of the screen.

Data Preparation

Please refer to the corresponding page.

Gaussian Settings

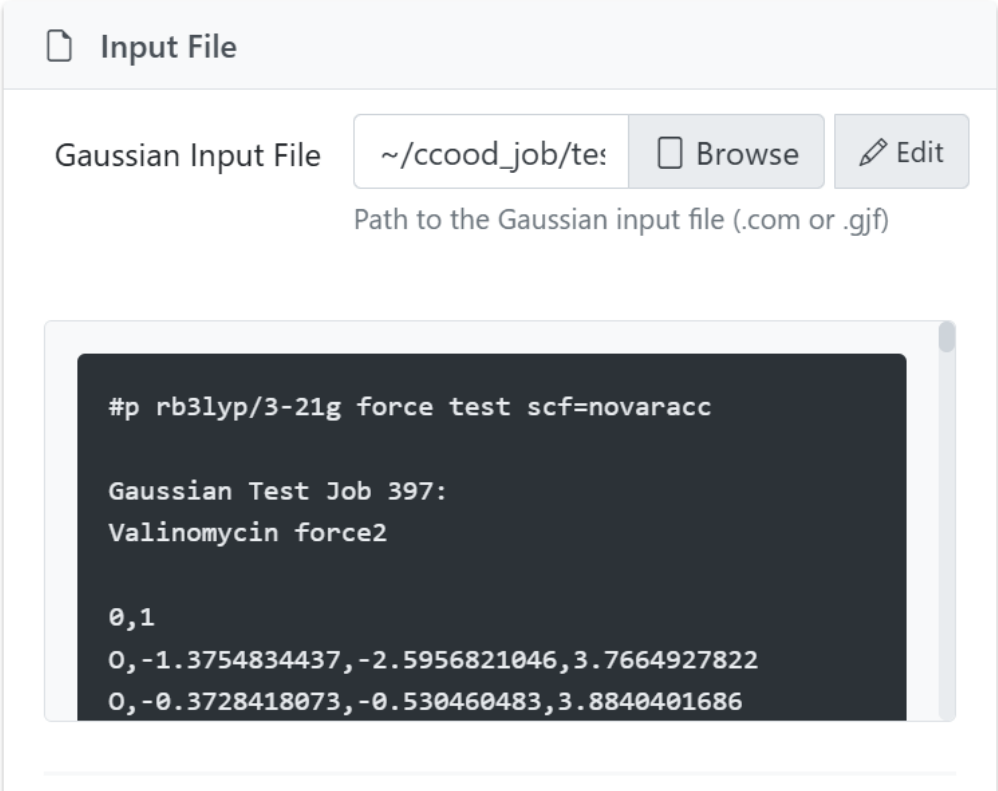
Input File Configuration

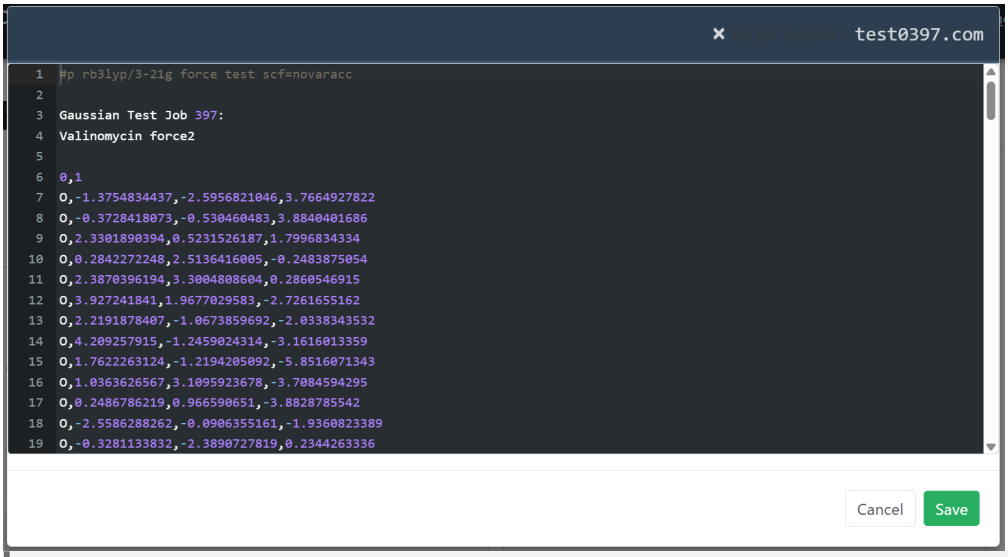
? File Selection

- Selection Method: Use the "Browse" button to open the file browser, or enter the file path directly
- Preview Function: The contents of the file will be displayed automatically after selection

? File Editing

- Integrated Editor: Click the "Edit" button to directly edit the input file
- Save: Click the "Save" button to save changes





Gaussian Version Selection

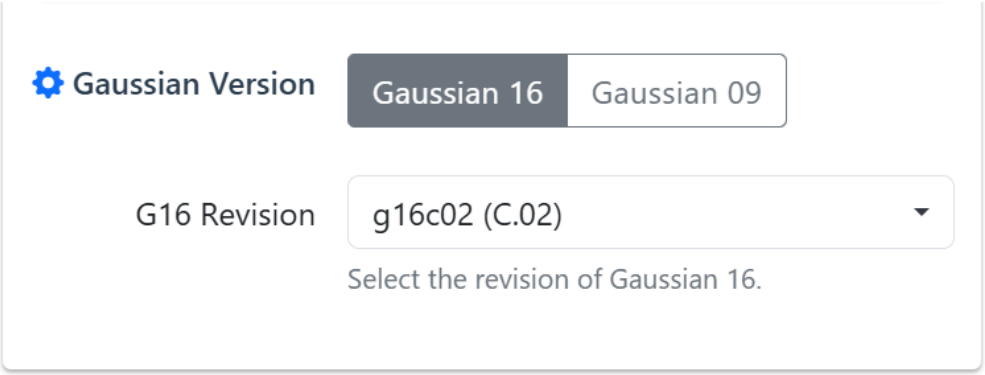
? Available Versions

Gaussian 16, Gaussian 09

? G16 Revision Selection

When Gaussian 16 is selected, choose from the following revisions:

c02, c01, b01



Computational Resource Settings

? Job Type Selection

Standard Computation

- 1–64 or 128 cores

Large-Memory Computation

- Use when standard memory is insufficient.
- Only 64 or 128 cores can be selected.

GPU Computation

- Not recommended due to limited speedup.
- Maximum 16 cores per GPU, up to a total of 128 cores.

? CPU Core Count Setting

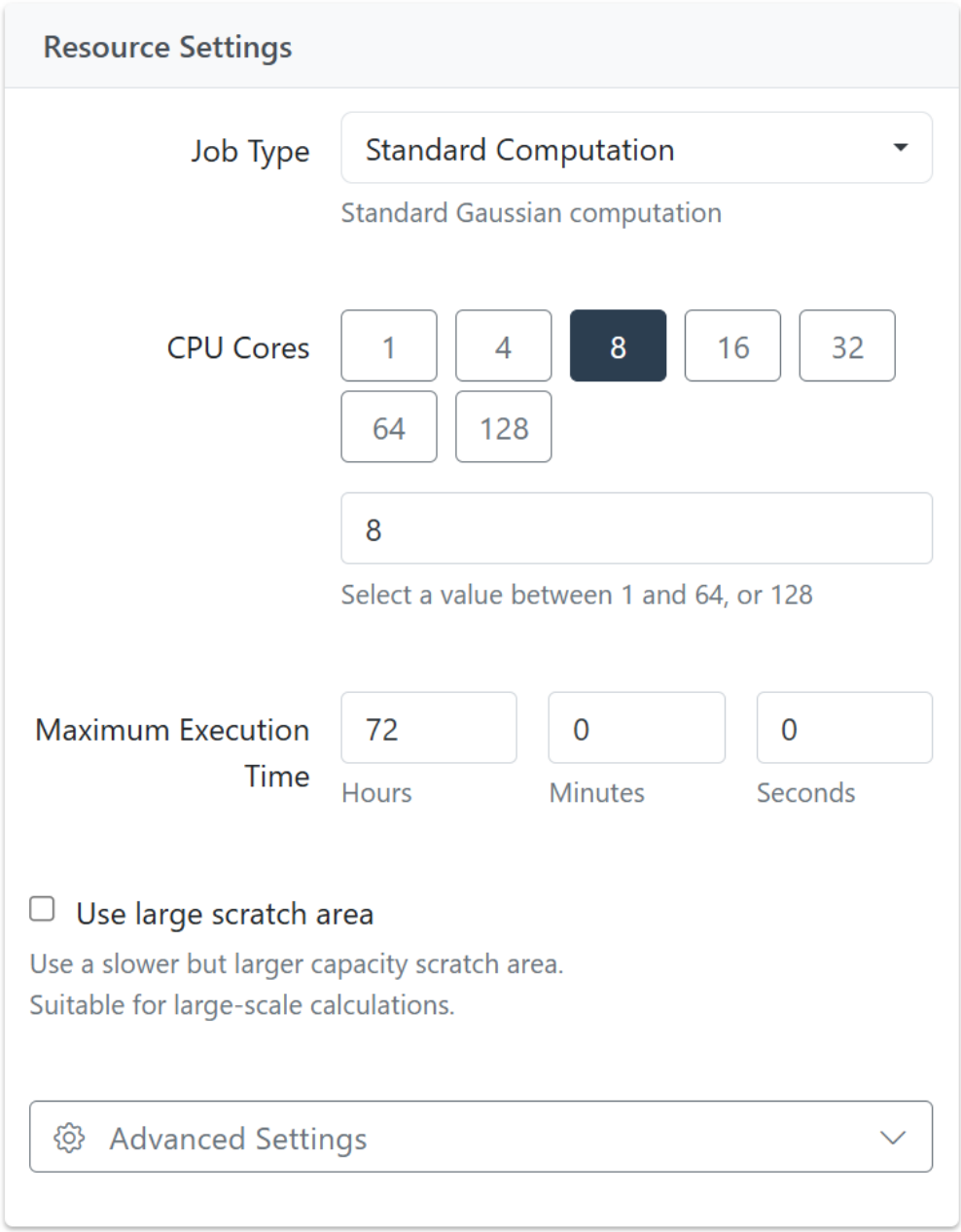
- Preset Selection: 1, 4, 8, 16, 32, 64, or 128 cores
- Manual Input: Enter any desired core count in the input field

? GPU Settings **(when GPU computation is selected): Set from 1 to 8 units**

? Wall Time Setting: Specify individually in hours, minutes, and seconds

? Storage Options

- Use the high-capacity `/gwork` directory as a scratch area
- Slightly slower performance



Advanced Settings (Optional)

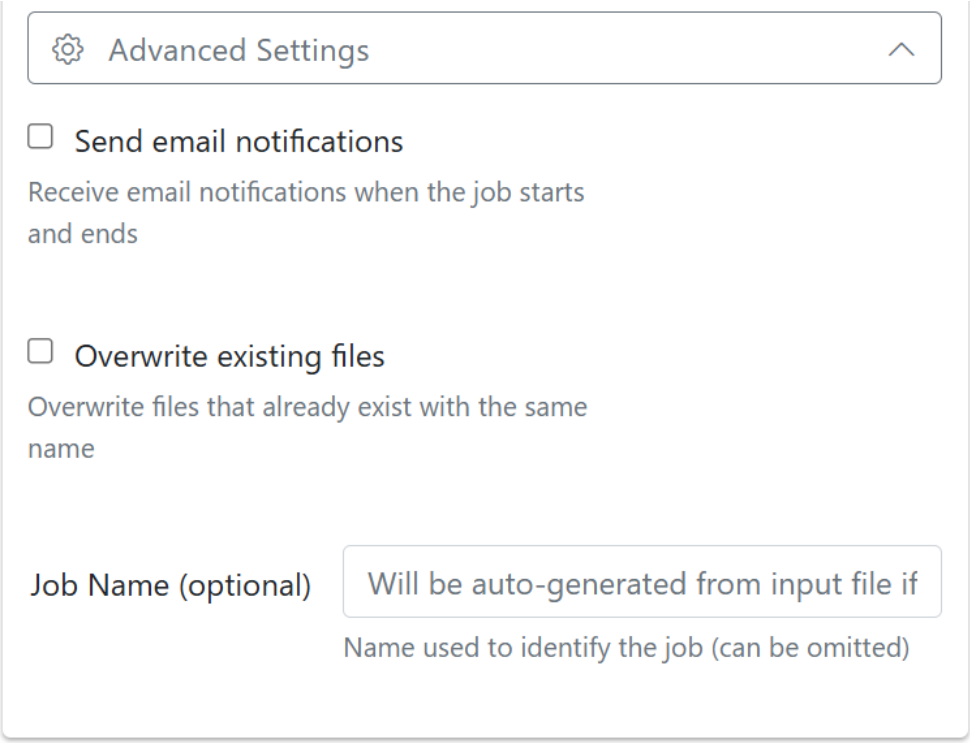
Click "Advanced Settings" to expand and configure the following options:

? Notification Settings: **Receive email notifications when the job starts and finishes**

? Overwrite Existing Files: **Set behavior when files with the same name already exist**

? Job Name Settings:

- Enter a custom job name
- If left blank, a name will be auto-generated from the input file (e.g., `test0397.com` → `test0397`)



Job Submission

Click the "Submit Job" button