



DOCUMENTATION

User Guide: Step by step user account configuration in WorkFlow

Key guides to orient yourself and get the most out of the platform from the beginning.

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WorkFlow

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WorkFlow

Welcome to WorkFlow:

In this guide we will show you step by step the user account configuration features in WorkFlow, we will review its operation in detail.

If you detect any bugs or errors within WorkFlow, please contact technical support to correct any anomalies that affect the operation within WorkFlow.

The names shown in this guide, such as titles, messages or lines of code, are illustrative examples only. It is not necessary to replicate them in experiments, as the values or inputs may vary from case to case.

TOOL GUIDE

Step 1 - Registration and Login

Account creation

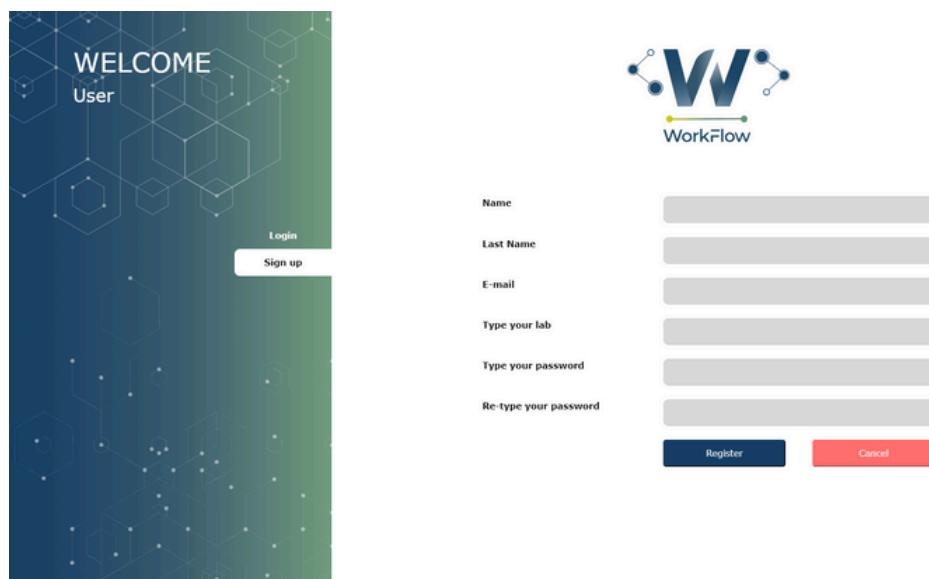
This document provides a step-by-step guide for the initial setup of WorkFlow, from registration to connecting to the workstation and setting up SSH keys.

Steps Figure 1:

Figure 1



Figure 2



Registration and Login:

- Go to <http://opaat.scripps.edu/>
- Click on "Sign Up" (located on the left side of the screen) **Figure 1 (A)**.
- Complete the registration form with your information.
- Click "Register". **Figure 2**
- Log in with your email and password.

TOOL GUIDE

Step 2: Workstation Profile Connection

Initial settings configuration

To connect WorkFlow to your workstation, follow these steps:

The screenshot shows the 'Initial settings configuration' step of the WorkFlow setup. At the top, there is a dropdown menu labeled 'Execution profile: Oppat'. To its right, a note says 'Select execution profile with you will bind your certificate'. Below this, there are two input fields: 'User name:' and 'Path:', both with placeholder text. To the right of the 'Path:' field is a note: 'Enter your SSH user and the path where your experiments will be saved.' A large blue callout box labeled 'A' points to the 'Path:' input field.

Execution profile: Oppat Select execution profile with you will bind your certificate

User name: Path: Enter your SSH user and the path where your experiments will be saved.

A

SSH KEY
Selected file: certificate
Select file No se han seleccionado archivos.

Complete the setup form:

- Select your workstation from the execution profile drop-down menu.
- Username: Enter your username on your server or workstation.
- Path: Define the directory where the workflow will run.

Note. For the Path field, we recommend adding “/workflow” to the end of the directory. This will ensure that the files generated by the workflow are kept in their own directory.

Please make sure that the path does not have any files or directories named workflow. Pre-existing files or directories with the name “workflow” will cause an error in this process.

It is recommended to use a specific path such as /home/testuser/workflow (A)

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Step 3: SSH key generation and configuration

To generate an SSH key, Run the following commands on your local machine:

- `$ ssh-keygen -t rsa -f workflow`
- Press Enter (leave the passphrase empty).
- Press Enter again (leave the confirmation empty).
- To copy the public key to your server/workstation, use the following command:
`$ ssh-copy-id -i workflow.pub your_username@your_worstation_url`
- SSH key: Upload the private key generated using `ssh-keygen`.

Important Notes:

Your private key will be named workflow (without .pub extension).

Upload this file in the SSH Key field of the WorkFlow configuration.

Association with user account

The screenshot shows a software interface for managing SSH keys. At the top, there is a dropdown menu labeled "Execution profile:" with "Oppat" selected. A tooltip next to it says "Select execution profile which you will bind your certificate". Below this, there are two input fields: "User name:" containing "testuser" and "Path:" containing "/home/testuser/workflow". To the right of these fields is a tooltip: "Enter your SSH user and the path where your experiments will be saved." At the bottom of the interface, there is a section titled "SSH KEY" with a sub-section "Selected file: certificate". Inside this section, there is a blue folder icon with a white "W" logo, indicating a selected file. Below the folder icon is a button labeled "Select file" and a message "No se han seleccionado archivos." (No files have been selected).

figure 1

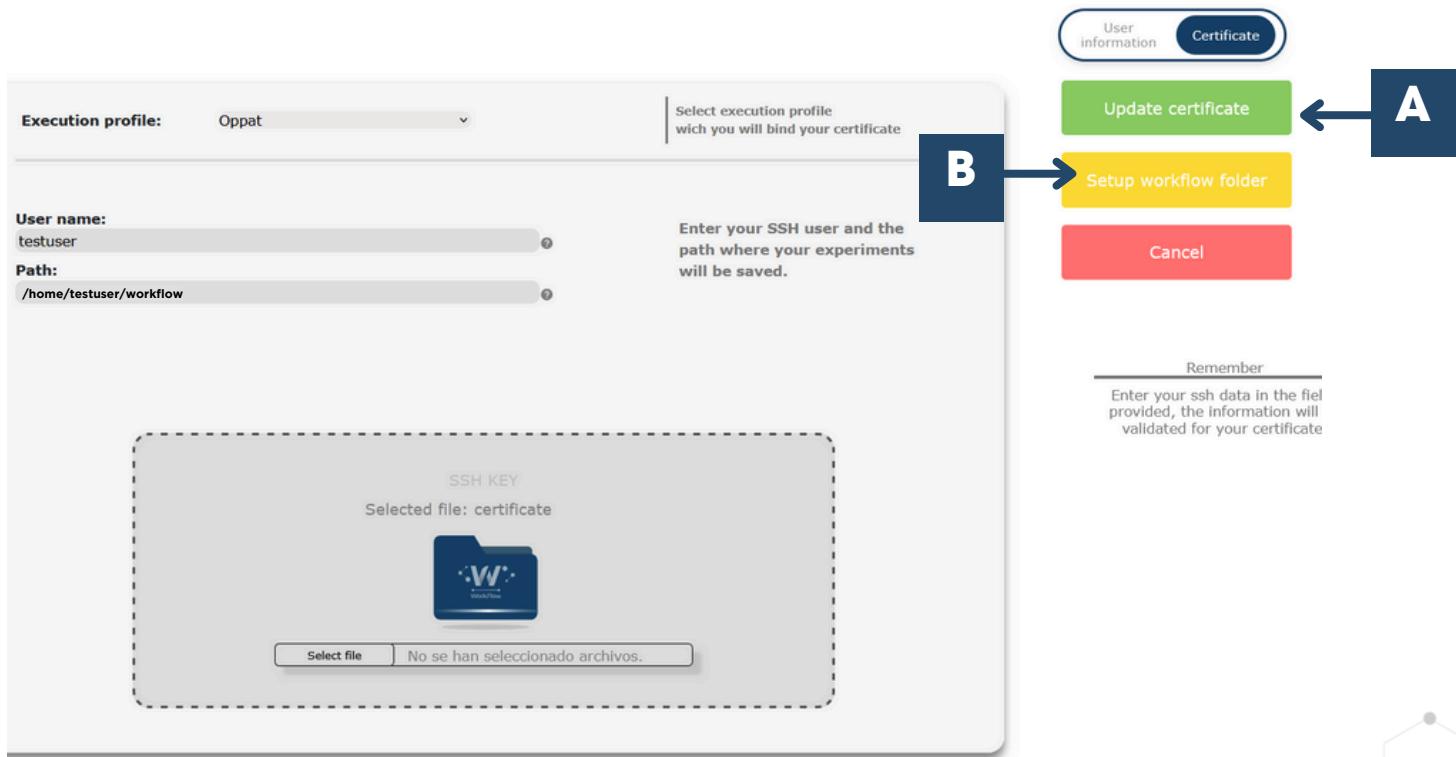
- In this way the form will have the following appearance, as shown in figure 1:

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• Step 4 - Confirmation and Termination

Configuration review

- After completing the form, click “Confirm Certificate” (located on the right side of the screen). (A)
- Once the process is complete, click on “Set Up Workflow Folder” to complete the configuration. (B)



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Step 5: Experiment set up

Experiment Location

To access the Sleep_WorkFlow experiment, go to the Experiments section and locate it in the Public WorkFlows table (Figure 1). By double-clicking on the experiment, you will be able to view all previous experiments performed within it. You can create a new experiment to perform the necessary tests (Figure 2).

Figure 1

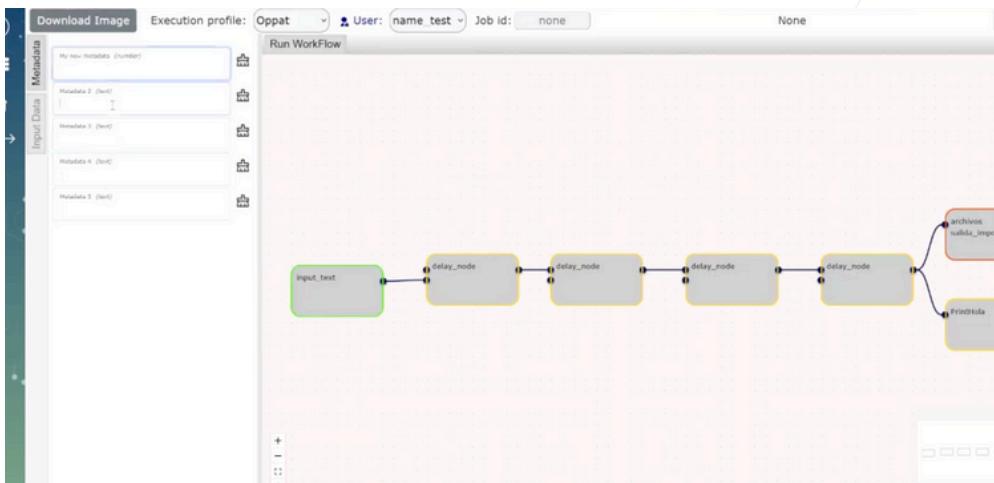


Figure 2

Name	Description	Author
WF_IO_NODE_PH_3_imported_3		name_te...
ModelAngelo	Runs modelangelo with default params.	Charles
Multiple_sequence_alignment	This workflow has the intention to develop a multiple sequence alignment	name_te...
sc6wao_ngs_analysis		Charles
sleep_workflow		name_te...

TOOL GUIDE

Figure 3



Experiment Setup

Metadata and Data Entry:

Inside the Run Workflow CANVA, on the left side, you will find five predefined metadata for the Sleep_Workflow experiment. To enter data, go to the Input Data section, located at the top right. (Figure 3)

Important: You must enter numeric values. If you enter text, the code will generate an error. For this guide, we will enter the numeric value 5.

Confirmation of saving:

To verify that the data has been saved correctly, check the top right of the screen. Click anywhere outside the input box to display the message.

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Entering metadata and data

In the Execution Profile section, verify the address is correct. This will allow the server to generate the code on the main server. If the experiment takes longer than expected to run, it is possible that the server is overloaded. (Figure 4)



Figure 4

Defining run parameters

Running the Experiment:

- When the program is compiled, all nodes will change color. The following states will appear in the top bar:

None: The program is paused. (Figure 5)

Submitted: The program is running. A pop-up message with the text “The experiment is ready to run” will be displayed, indicating that the information has been sent. (Figure 6)

Running: The program is in the process of execution. (Figure 7)

Finished: The execution is finished. If no errors were found, all nodes will appear green. (Figure 8)

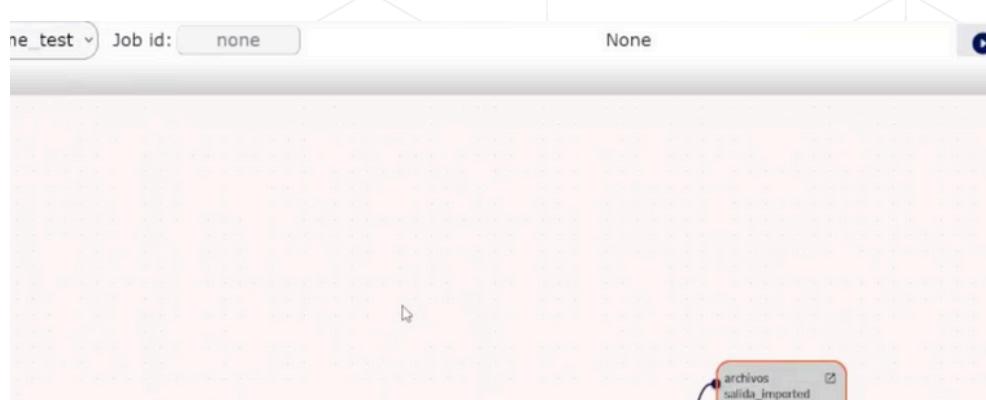


Figure 5

TOOL GUIDE

Start of the process

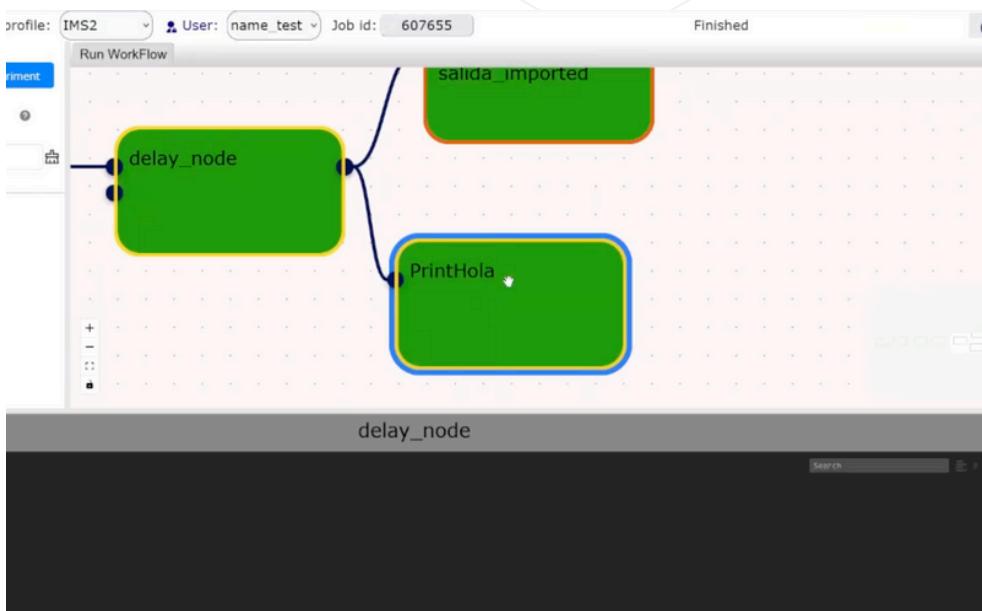
Figure 6



Figure 7



Figure 8

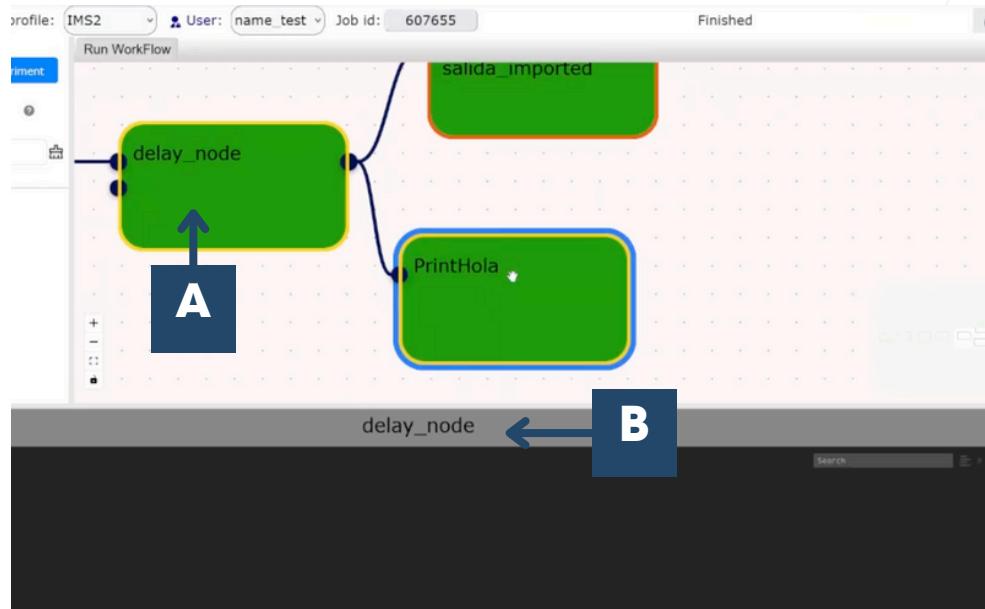


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Node Identification

Each time you select a node, its name will appear in the gray bar of the console. (Figure 1)

Figure 1



- Selected node (A)
- Gray bar with the name of the node you have selected (B)

Note: You must click on Stdout Node or Stderr Node for the console to appear. Also click on the Stdout Node or Stderr Node to remove it from the window.

TOOL GUIDE

Downloading of results and graphs

Before finishing, go to the output_imported files node to view its contents.
Click on the output/enlarge view icon to view the generated graphs Figure 1.

Figure 1

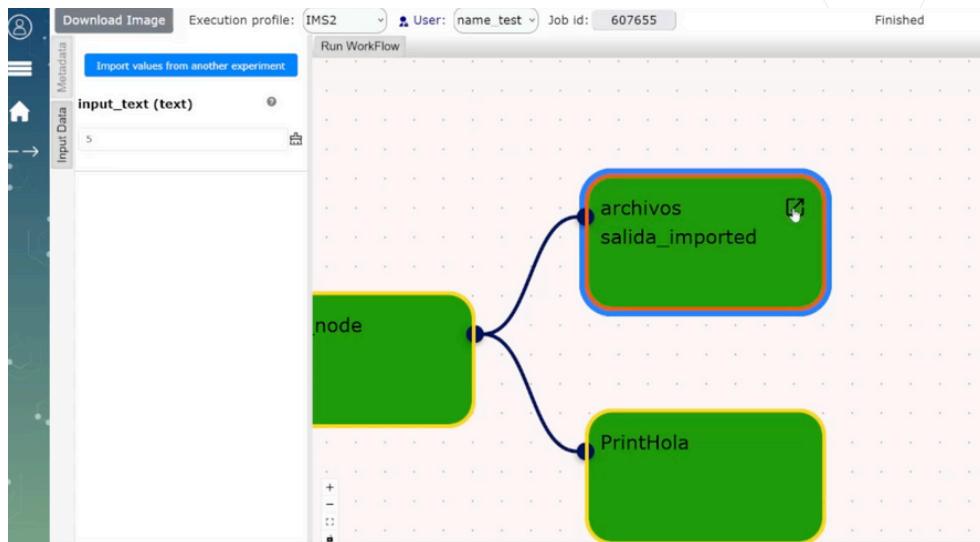


Figure 2

The screenshot shows a web browser window with several download links:

- A large blue square labeled 'Download File'.
- A link labeled 'mihtml.html'.
- A link labeled 'miarchivo.html' containing code for generating a Gif file.
- A link labeled 'Grafica de ejemplo' showing a graph of $y = x^2$.
- A table with columns 'Edad' and 'Ciudad' containing data:

Edad	Ciudad
10	New York
20	Los Ang...
30	Chicago

A black arrow points from the text 'To download the outputs click on "Download File", Files will be downloaded to your local computer Figure 2 (A).'

Downloading outputs

- To download the outputs click on "Download File", Files will be downloaded to your local computer Figure 2 (A).

TOOL GUIDE

Step 6: Workflow considerations and purpose of the experiment

Process evaluation

With these steps, your WorkFlow environment will be properly configured and ready for use. The Sleep_WorkFlow experiment is used to corroborate the correct operation of the WorkFlow system.

Important:

- *Make sure that the execution profile is well defined to avoid conflicts.*
- *Use descriptive and well-structured names to facilitate WorkFlow administration.*
- *Keep your SSH key secure and do not share it with other users.*
- *The nodes change color correctly.*
- *The connections between nodes are properly established.*
- *The generated graphs are displayed and work correctly.*



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Thank you

This concludes this lesson. If you have any questions, consult your leader to resolve any concerns.