Using Interactive Development Environments (Jupyter, VS Code)

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Desktop Environment

OpenOnDemand's desktop environment allows you to use applications through a graphical interface (GUI).

Main Uses:

- Using GUI-based software such as GaussView
- · Intuitive file operations using file manager



Starting a Session

ktop	Desktop (launched-by-o 7ffd71d6f12a@ccfep1)	ndemand-af99baad-e406-49a7-9f58- 1 node 1 core Run	
app will launch an interactive desktop on one or more oute nodes. You will have full access to the resources a nodes provide. This is analogous to an interactive a job. ber of hours	Host: >_ ccfep1.center.ims.ac.jp Created at: 2025-01-31 17:14:41 JST Time Used: less than 1 minute Session ID: 04911667-409a-4f2b-8277-7396dd9be04e		
	Compression	Image Quality	
Launch	0 (low) to 9 (high)	0 (low) to 9 (high)	
Desktop session data for this session can be accessed	Launch Desktop	View Only (Share-able	

- 1. Click the "Desktop" icon from the dashboard
- 2. Configure the following in the session settings:
- Number of hours: Specify usage time 3. Click the [Launch] button
- 4. Once session preparation is complete, click [Launch Desktop]

Session Management

- Running desktop sessions can be viewed in "My Interactive Sessions" on the dashboard
- To end a session, click "Delete" for the corresponding session in "My Interactive Sessions"

Important Notes

- Sessions are maintained even if you accidentally close the browser tab. You can reconnect via "Launch Desktop"
- Sessions automatically end after the specified usage time
- Please end sessions promptly after use for efficient resource utilization

Using GaussView

You can launch GaussView using the OpenOnDemand desktop environment.

How to Launch GaussView

- 1. Log in to the OpenOnDemand desktop environment
- 2. Open a terminal on the desktop



3. Enter the following command to launch GaussView:

gview6

4. The GaussView main window will appear

Jupyter Notebook

Jupyter Notebook is an interactive development environment that allows you to combine program code, execution results, and explanatory text in a single notebook format. It supports various programming languages, including Python.

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B + %	□ □ ► ■ C ► Code ∽ JupyterLab □	ø	Pytho	n 3 (ipy	kernel)) C
[18]:	<pre>plt.figure(figsize=(6, 4)) plt.plot(wavelengths, spectrum, 'b-', alpha=0.5, label='Raw Data') plt.plot(wavelengths, smoothed_spectrum, 'r-', label='Smoothed') plt.vlabel('Wavelength (nm)') plt.ylabel('Absorbance') plt.title('UV-Vis Spectrum Analysis') plt.legend() plt.gend() plt.geid(True, alpha=0.3) plt.tight_layout() plt.show()</pre>	\uparrow	\downarrow	± ₽		
	UV-Vis Spectrum Analysis					

Basic Usage

Starting a Session

- 1. Click the "Jupyter Notebook" icon from the OpenOnDemand dashboard
- 2. Specify the following in the settings screen:
 - Number of hours: Session duration (in hours)
- 3. Click the "Launch" button
- Once ready, click "Connect to Jupyter"

 Jupyter environment opens in a new tab

Creating a New Notebook

- 1. Click the "New" button in the top right
- 2. Select programming language/runtime environment:
- Choose desired environment from the list
- Default is "Python3 (ipykernel)": Python 3.10 environment from /apl/conda/20240305

	- New ≜Upload C
	dza_venv
	dza_python_env
La	R
	📕 JavaScript (Node.js)
	💻 dza_conda
	Python 3 (ipykernel)
	s_ Terminal
	Console
	📃 New File
	New Folder

Note: You can switch to a different runtime environment from the menu in the top right even after creation.

Additional note: The runtime environment selected here is called a "kernel". Custom environment setup is explained in the "Customizing Python Environment" section.

Basic Notebook Operations

About Cells

Notebooks consist of blocks called "cells". There are several types:

- Code: Area for writing and executing programs
- Markdown: Area for explanatory text (can be formatted using Markdown)
- Raw: Area for plain text without formatting

Basic Operations

Cell Operations:

- Add new cell: [+] button at top
- Change cell type: Select "Code", "Markdown", etc. from toolbar dropdown
- Execute cell: Shift + Enter (or ► button)
 - Code: Program executes and displays results
- Markdown: Formatted text is displayed
- Select cell: Click cell (blue border appears)

Other Operations:

- Save file: Ctrl + S or save icon at top
- Delete cell: Select cell and press D key twice
- Check execution order: View numbers on left side of cells

Customizing Python Environment

Default Environment

Default Python environment (Python 3.10) from /apl/conda/20240305 is available * All Python packages installed in this environment are ready to use

Steps to Add Custom Environment

To use your own Python environment in Jupyter, follow these steps in the shell:

For Conda environments:



Install ipykernel pip install ipykernel pip install <required-package-names>

Register as Jupyter kernel python -m ipykernel install --user --name myenv --display-name "My Python Env"

Once registered, the added kernel becomes available for selection.

Important Notes

- You can reconnect through "My Interactive Sessions" if you accidentally close the browser tab
- · Sessions automatically end after the specified usage time

VS Code (Code Server)

VS Code is a feature-rich code editor that enables efficient programming and text editing. It integrates essential development features including file editing, program execution, and debugging.

Basic Usage

Starting a Session

- 1. Click "Code Server" icon from OpenOnDemand dashboard
- 2. Specify in settings screen:
 - Number of hours: Specify session time (in hours)
 - Working Directory: Specify working directory
 - * Default is home directory (\$HOME)
 - * Can select different directory with "Select Path" button
 - Codeserver Version : Select version
 - * Latest version (4.8) recommended unless otherwise needed
- 3. Click "Launch" button
- 4. Once ready, click "Connect to VS Code" \rightarrow VS Code environment opens in new tab

Basic Screen Layout

- · Left sidebar: Access various functions including file list and extensions
- Main editor: File editing area
- Bottom panel: Display terminal, output, debug information, etc.



- Open file:
 - Click file in sidebar file explorer
 - Or Ctrl + O to select file
- Save file: Ctrl + S
- Create new file: Ctrl + K N

Using Terminal

Command line operations available via terminal:

- Open terminal:
 - Select [Terminal] → [New Terminal] from menu
 - Or Ctrl + ` (backtick)
- Multiple terminals:
 - New terminal: [+] button
 - Split terminal: [Split Terminal] icon
 - Switch terminals: Use menu on right of terminal panel

Extensions

VS Code allows installation of extensions as needed. Installed extensions persist after session ends.

- 1. Click Extensions icon (four squares) in sidebar
- 2. Enter extension name or keyword in search bar
- 3. Click [Install] on desired extension

Useful Features

- Command palette: Ctrl + Shift + P
 Quick access to all VS Code functions
- Find in file: Ctrl + F
- Find in project: Ctrl + Shift + F

Important Notes

- You can reconnect through "My Interactive Sessions" if you accidentally close the browser tab
- · Sessions automatically end after the specified usage time