Integrating an IDE with HTCondor

With the example of Visual Studio Code

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26th September, 2024

Physics Institute at University of Bonn

- over 280 members in 28 working groups, plus users from related Physics institutes and with HTC workloads
- Biggest particle accelerator run by a German university ('ELSA', 164.4 m circumference) with two experiments ($\approx$ 50 people)
- Groups from:
  - particle physics: ATLAS, Belle II, COMPASS/AMBER, Alice, LHCb, ...
  - hadron physics
  - detector development
  - photonics
  - theory groups
  - economics

Extremely diverse requirements on software environments & job resources.

since 2017: **HTCondor** with **interactive-first** concept

‘Interactive First’

- Scientific software tends to require more and more dependencies (user-defined software stacks)
  ⇒ often via containers, Python environments, CVMFS trees,. . .
- Users do not want to hassle with the setup on their desktop, on which they prefer to use a modern OS
  ⇒ Decent versions of IDEs, graphics editors, browsers etc.

Solutions

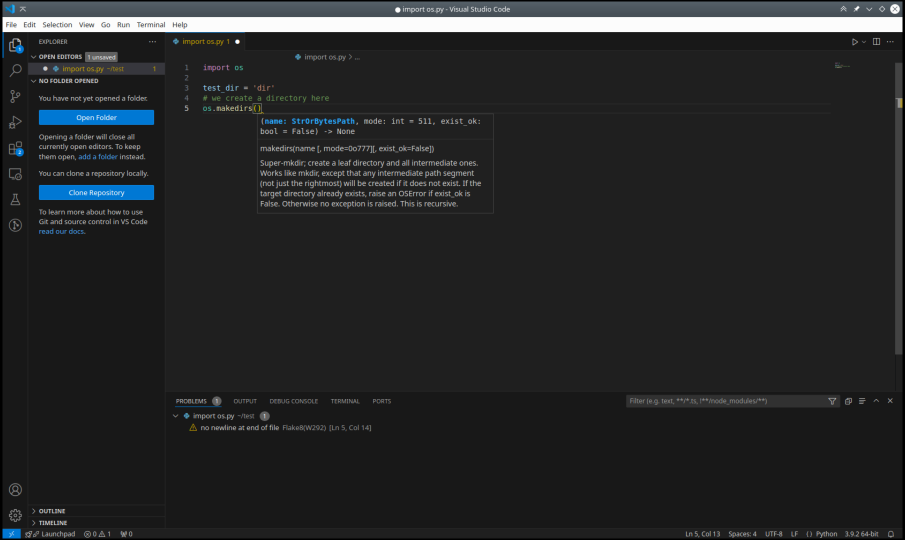
Two talks will highlight our approaches:

- Oliver: `SSH` into containers on Batch resources and JupyterHub on Batch resources
- Myself: Using an IDE to `SSH` into containers on Batch resources

Why Visual Studio Code?

- Gained a lot of popularity over the last years among our users
- (Probable) reasons for its popularity:
  - Syntax highlighting for most widely spread coding languages
  - Easy to install extensions ⇒ easily customisable
  - Brings own ‘terminal’ where you can run your code without leaving the IDE
- Goal: offer a way to develop code with VS Code while being able to test it in the Batch environment

Why Visual Studio Code?


● import os.py - Visual Studio Code
File Edit Selection View Go Run Terminal Help
EXPLORER
OPEN EDITORS 1 unsaved
● import os.py ~/test 1
NO FOLDER OPENED
Open Folder
Clone Repository
import os.py 1 ●
import os.py > ...
PROBLEMS 1 OUTPUT DEBUG CONSOLE TERMINAL PORTS
Filter (e.g. text, **/*.ts, !**/node_modules/**)
OUTLINE
TIMELINE
Launchpad ⊗ 0 ⚠ 1 0
Ln 5, Col 13 Spaces: 4 UTF-8 LF {} Python 3.9.2 64-bit

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To learn more about how to use Git and source control in VS Code read our docs.

```
import os

test_dir = 'dir'
# we create a directory here
os.makedirs()
```

```
(name: StrOrBytesPath, mode: int = 511, exist_ok:
bool = False) -> None
```

makedirs(name [, mode=0o777][, exist_ok=False])

Super-mkdir; create a leaf directory and all intermediate ones. Works like mkdir, except that any intermediate path segment (not just the rightmost) will be created if it does not exist. If the target directory already exists, raise an OSError if exist_ok is False. Otherwise no exception is raised. This is recursive.

```
import os.py ~/test 1
  ⚠ no newline at end of file Flake8(W292) [Ln 5, Col 14]
```

What do we want to achieve?

Key questions

- Where to best run VS Code? Inside/outside the job?
- How to prevent long-running editing sessions that might go stale and block ressources?
- How to get the user's code into these jobs?

Key requirements

- Need answers that result in a workflow which feels as 'natural' as possible
- As little administrative maintenance as possible
- We need some kind of monitoring

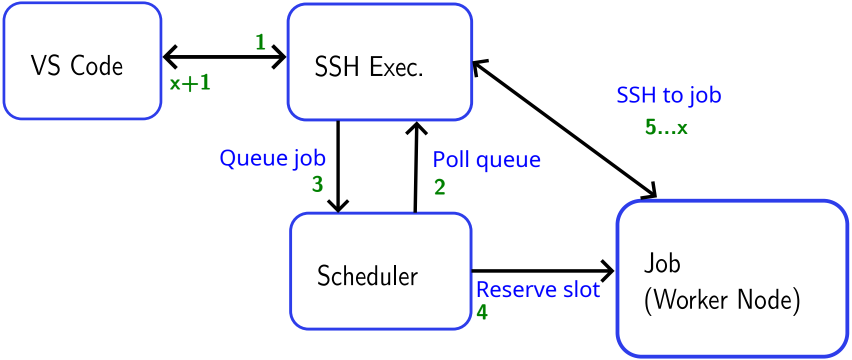
Our approach

- Make use of VS Code's ‘Remote SSH’-Plugin
  - Start an ‘interactive’ batch job from your IDE
  - Feels like SSH-ing to another host
- This way we do not need to install VS Code on Worker Nodes
  - Binaries built by Microsoft are not distributable (licensing)
  - We cannot use VS Codium because we need Microsoft's ‘Remote SSH’-Plugin
- Everything is set up on the client's side
- What do we actually need for this approach?
  - A new job flavor to set defaults, constraints and for monitoring
  - A custom `SSH` executable to use from VS Code

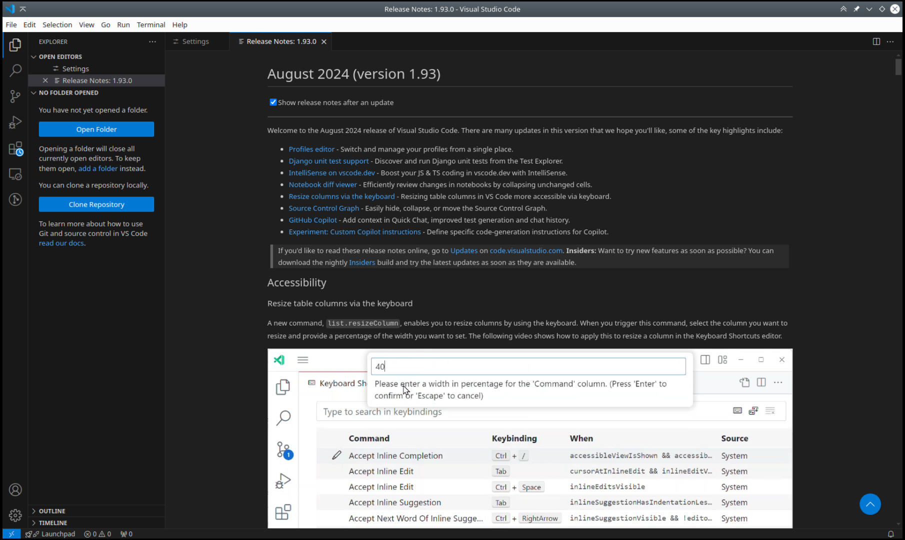
Custom SSH executable

- VS Code's 'Remote SSH'-Plugin expects an `SSH` executable
  - We need to 'emulate' such an executable
  - Within this executable we need to start and connect to a batch job
- General idea:
  - Write a Python executable
  - Use HTCondor's Python API to submit and connect to a batch job
  - Allow only one Editing job per submit host
- Need to take care to handle options passed to `condor_ssh_to_job`
- Need to wrap input / output while job is in queue and not yet started

Custom SSH executable



Seeing it in action



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Open Folder

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Clone Repository

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August 2024 (version 1.93)

☑ Show release notes after an update

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- Profiles editor - Switch and manage your profiles from a single place.
- Django unit test support - Discover and run Django unit tests from the Test Explorer.
- IntelliSense on vscode.dev - Boost your JS & TS coding in vscode.dev with IntelliSense.
- Notebook diff viewer - Efficiently review changes in notebooks by collapsing unchanged cells.
- Resize columns via the keyboard - Resizing table columns in VS Code more accessible via keyboard.
- Source Control Graph - Easily hide, collapse, or move the Source Control Graph.
- GitHub Copilot - Add context in Quick Chat, improved test generation and chat history.
- Experiment: Custom Copilot instructions - Define specific code-generation instructions for Copilot.

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Accessibility

Resize table columns via the keyboard

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40

Please enter a width in percentage for the 'Command' column. (Press 'Enter' to confirm or 'Escape' to cancel)

Type to search in keybindings

Command	Keybinding	When	Source
Accept Inline Completion	Ctrl + /	accessibleViewIsShown && accessib...	System
Accept Inline Edit	Tab	cursorAtInlineEdit && inlineEditV...	System
Accept Inline Edit	Ctrl + Space	inlineEditsVisible	System
Accept Inline Suggestion	Tab	inlineSuggestionHasIndentationLes...	System
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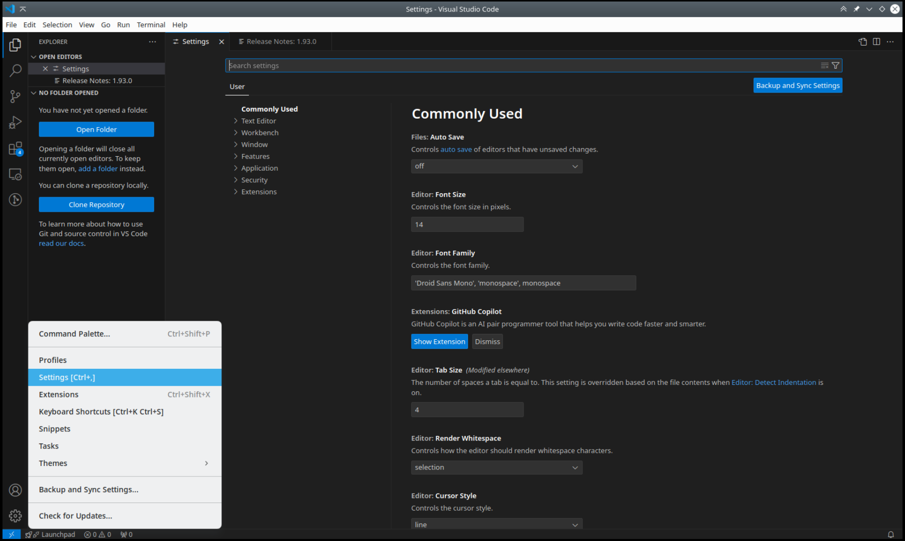
Seeing it in action



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Commonly Used

Files: Auto Save
Controls auto save of editors that have unsaved changes.
off

Editor: Font Size
Controls the font size in pixels.
14

Editor: Font Family
Controls the font family.
'Droid Sans Mono', 'monospace', monospace

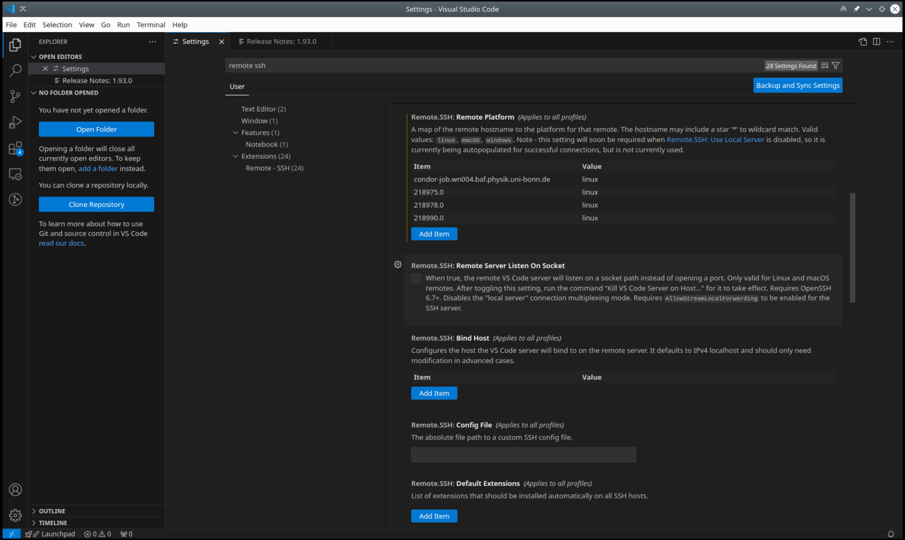
Extensions: GitHub Copilot
GitHub Copilot is an AI pair programmer tool that helps you write code faster and smarter.

Editor: Tab Size *(Modified elsewhere)*
The number of spaces a tab is equal to. This setting is overridden based on the file contents when Editor: Detect Indentation is on.
4

Editor: Render Whitespace
Controls how the editor should render whitespace characters.
selection

Editor: Cursor Style
Controls the cursor style.
line

Seeing it in action



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Remote.SSH: Remote Platform *(Applies to all profiles)*

A map of the remote hostname to the platform for that remote. The hostname may include a star '*' to wildcard match. Valid values: `linux`, `macOS`, `windows`. Note - this setting will soon be required when Remote.SSH: Use Local Server is disabled, so it is currently being autopopulated for successful connections, but is not currently used.

Item	Value
condor-job.wn004.baf.physik.uni-bonn.de	linux
218975.0	linux
218978.0	linux
218990.0	linux

Remote.SSH: Remote Server Listen On Socket

□ When true, the remote VS Code server will listen on a socket path instead of opening a port. Only valid for Linux and macOS remotes. After toggling this setting, run the command "Kill VS Code Server on Host..." for it to take effect. Requires OpenSSH 6.7+. Disables the "local server" connection multiplexing mode. Requires `AllowStreamLocalForwarding` to be enabled for the SSH server.

Remote.SSH: Bind Host *(Applies to all profiles)*

Configures the host the VS Code server will bind to on the remote server. It defaults to IPv4 localhost and should only need modification in advanced cases.

Item	Value

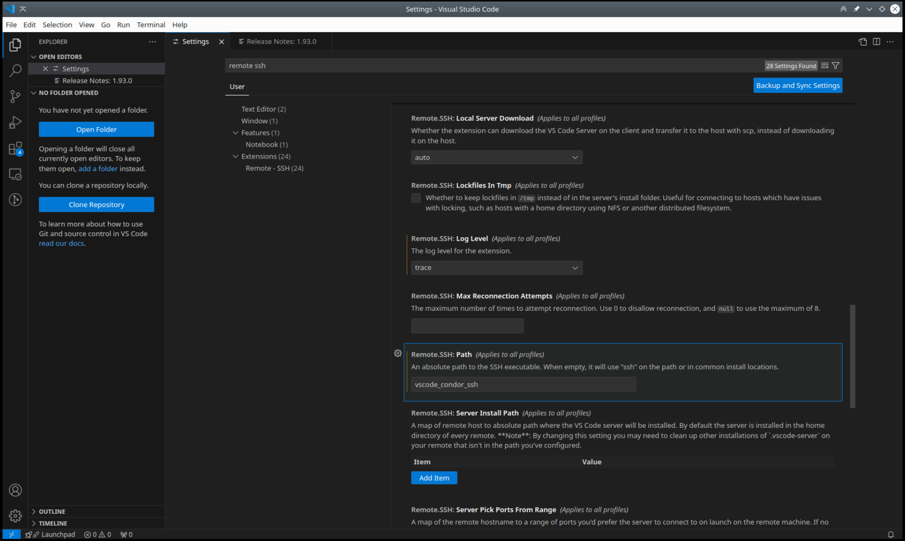
Remote.SSH: Config File *(Applies to all profiles)*

The absolute file path to a custom SSH config file.

Remote.SSH: Default Extensions *(Applies to all profiles)*

List of extensions that should be installed automatically on all SSH hosts.

Seeing it in action



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remote ssh

Remote.SSH: Local Server Download *(Applies to all profiles)*
Whether the extension can download the VS Code Server on the client and transfer it to the host with scp, instead of downloading it on the host.
auto

Remote.SSH: Lockfiles In Tmp *(Applies to all profiles)*
□ Whether to keep lockfiles in `/tmp` instead of in the server's install folder. Useful for connecting to hosts which have issues with locking, such as hosts with a home directory using NFS or another distributed filesystem.

Remote.SSH: Log Level *(Applies to all profiles)*
The log level for the extension.
trace

Remote.SSH: Max Reconnection Attempts *(Applies to all profiles)*
The maximum number of times to attempt reconnection. Use 0 to disallow reconnection, and `null` to use the maximum of 8.

Remote.SSH: Path *(Applies to all profiles)*
An absolute path to the SSH executable. When empty, it will use "ssh" on the path or in common install locations.
vscode_condor_ssh

Remote.SSH: Server Install Path *(Applies to all profiles)*
A map of remote host to absolute path where the VS Code server will be installed. By default the server is installed in the home directory of every remote. **Note**: By changing this setting you may need to clean up other installations of `.vscode-server` on your remote that isn't in the path you've configured.

Remote.SSH: Server Pick Ports From Range *(Applies to all profiles)*
A map of the remote hostname to a range of ports you'd prefer the server to connect to on launch on the remote machine. If no

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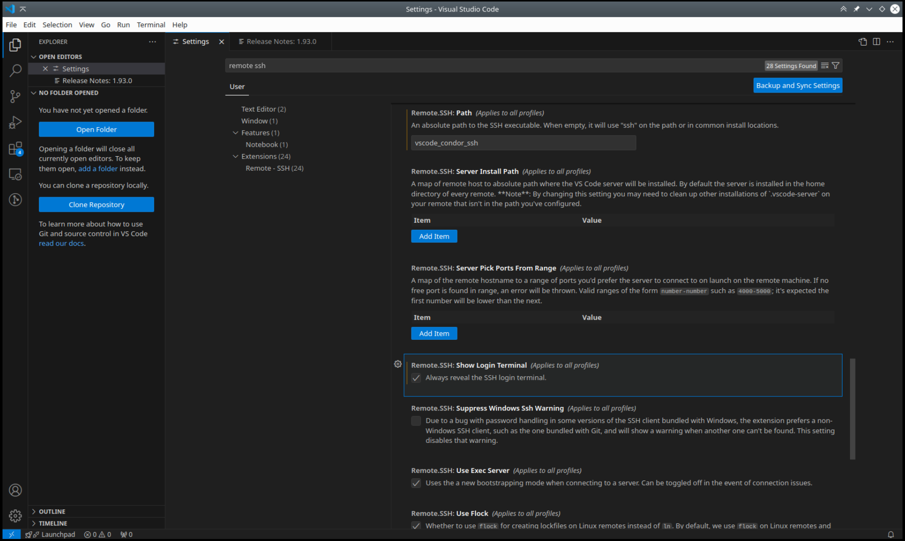
Seeing it in action



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Item	Value

Add Item

Remote.SSH: Server Pick Ports From Range *(Applies to all profiles)*

A map of the remote hostname to a range of ports you'd prefer the server to connect to on launch on the remote machine. If no free port is found in range, an error will be thrown. Valid ranges of the form `number-number` such as `4000-5000`; it's expected the first number will be lower than the next.

Item	Value

Add Item

Remote.SSH: Show Login Terminal *(Applies to all profiles)*

☑ Always reveal the SSH login terminal.

Remote.SSH: Suppress Windows Ssh Warning *(Applies to all profiles)*

☐ Due to a bug with password handling in some versions of the SSH client bundled with Windows, the extension prefers a non-Windows SSH client, such as the one bundled with Git, and will show a warning when another one can't be found. This setting disables that warning.

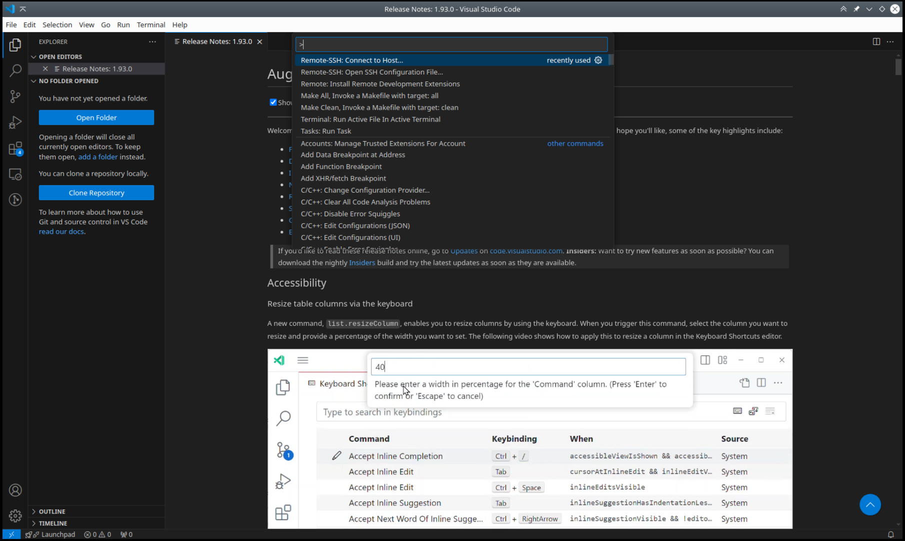
Remote.SSH: Use Exec Server *(Applies to all profiles)*

☑ Uses the a new bootstrapping mode when connecting to a server. Can be toggled off in the event of connection issues.

Remote.SSH: Use Flock *(Applies to all profiles)*

☑ Whether to use `flock` for creating lockfiles on Linux remotes instead of `ln`. By default, we use `flock` on Linux remotes and

Seeing it in action


Release Notes: 1.93.0 - Visual Studio Code
File Edit Selection View Go Run Terminal Help
EXPLORER
OPEN EDITORS
Release Notes: 1.93.0
NO FOLDER OPENED
Open Folder
Clone Repository
OUTLINE
TIMELINE
Launchpad ⊗ 0 ⚠ 0 ⑃ 0
Release Notes: 1.93.0
>
Remote-SSH: Connect to Host... recently used
Remote-SSH: Open SSH Configuration File...
Remote: Install Remote Development Extensions
Make All, Invoke a Makefile with target: all
Make Clean, Invoke a Makefile with target: clean
Terminal: Run Active File In Active Terminal
Tasks: Run Task
Accounts: Manage Trusted Extensions For Account other commands
Add Data Breakpoint at Address
Add Function Breakpoint
Add XHR/fetch Breakpoint
C/C++: Change Configuration Provider...
C/C++: Clear All Code Analysis Problems
C/C++: Disable Error Squiggles
C/C++: Edit Configurations (JSON)
C/C++: Edit Configurations (UI)
Aug
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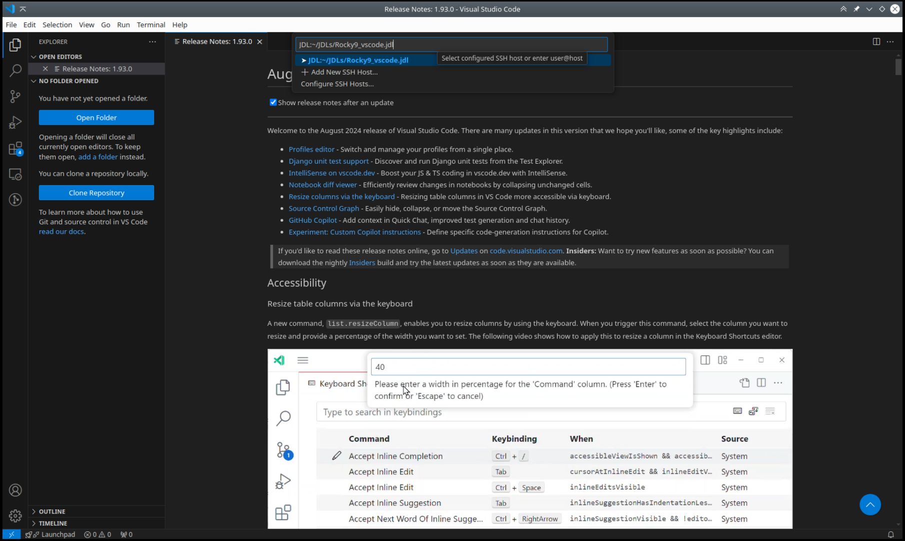

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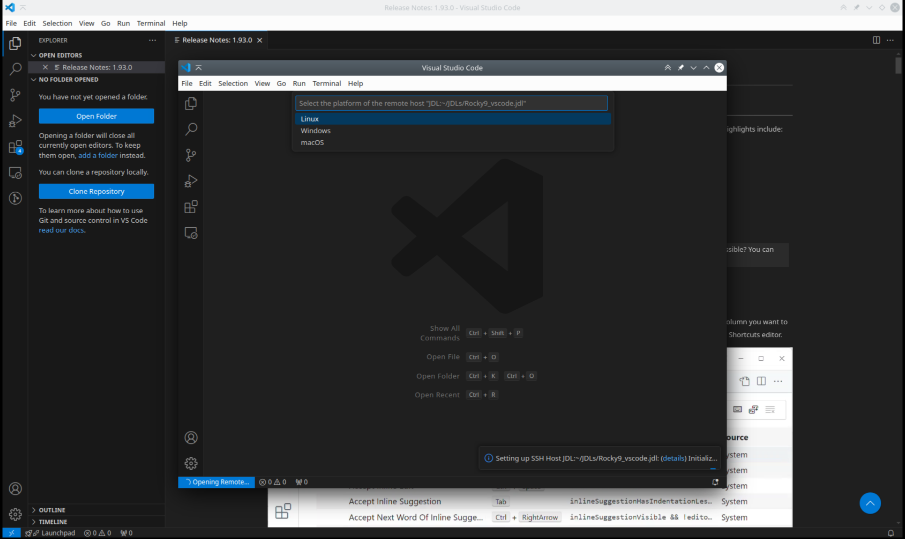

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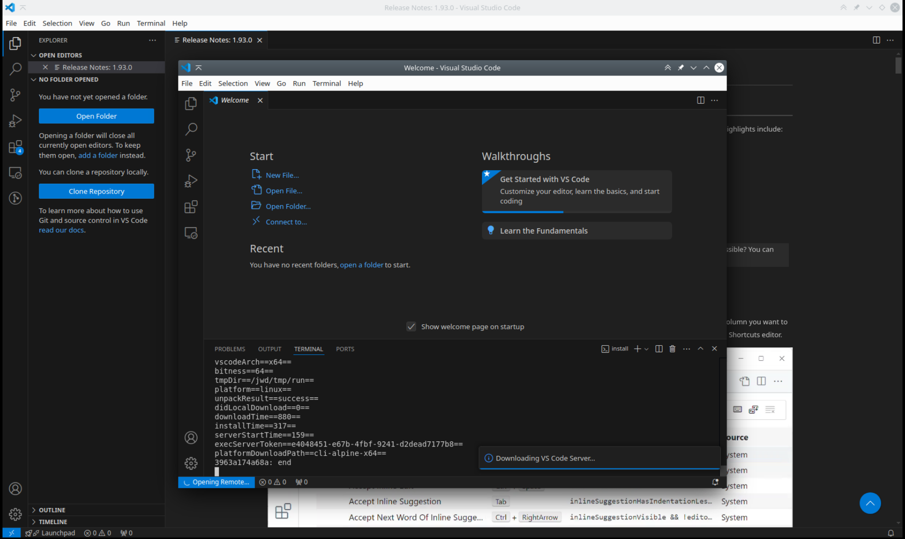
Select the platform of the remote host "JDL:~/JDLs/Rocky9_vscode.jdl"

Setting up SSH Host JDL:~/JDLs/Rocky9_vscode.jdl: (details) Initializ...

Accept Inline Suggestion	Tab	inlineSuggestionHasIndentationLes...	System
Accept Next Word Of Inline Sugge...	Ctrl + RightArrow	inlineSuggestionVisible && !edito...	System

Seeing it in action



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Customize your editor, learn the basics, and start coding

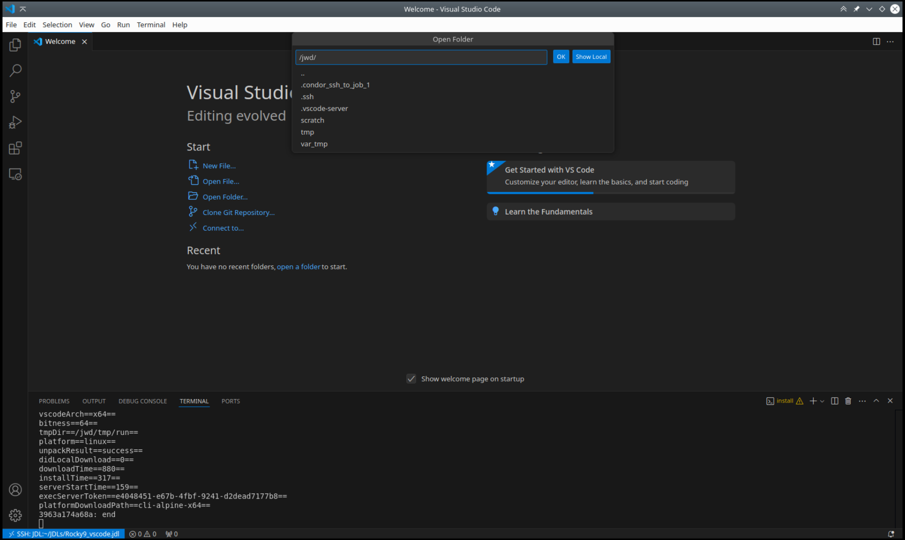
You have no recent folders, open a folder to start.

☑ Show welcome page on startup

```
vscodeArch==x64==
bitness==64==
tmpDir==/jwd/tmp/run==
platform==linux==
unpackResult==success==
didLocalDownload==0==
downloadTime==880==
installTime==317==
serverStartTime==159==
execServerToken==e4048451-e67b-4fbf-9241-d2dead7177b8==
platformDownloadPath==cli-alpine-x64==
3963a174a68a: end
```

Downloading VS Code Server...

Seeing it in action



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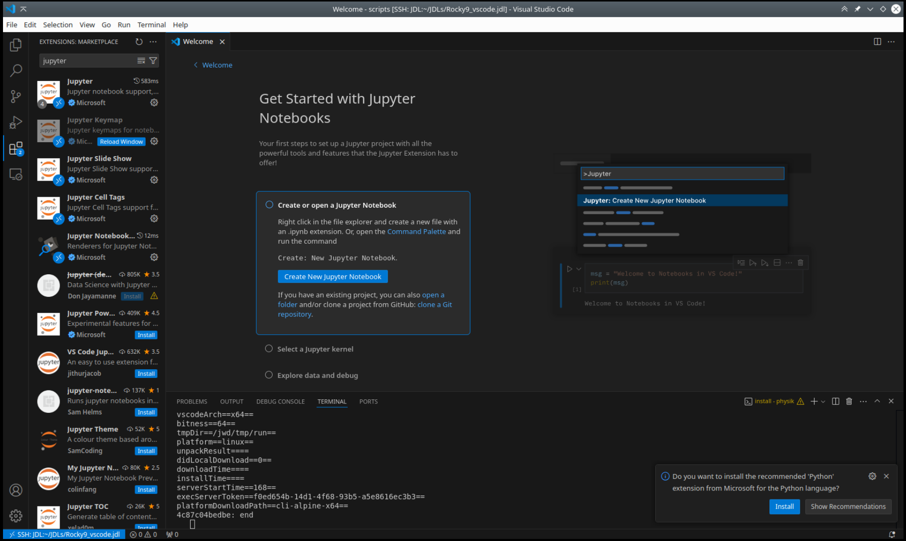
```
vscodeArch==x64==
bitness==64==
tmpDir==/jwd/tmp/run==
platform==linux==
unpackResult==success==
didLocalDownload==0==
downloadTime==880==
installTime==317==
serverStartTime==159==
execServerToken==e4048451-e67b-4fbf-9241-d2dead7177b8==
platformDownloadPath==cli-alpine-x64==
3963a174a68a: end
```

Seeing it in action



Welcome - scripts [SSH: JDL:~/JDLs/Rocky9_vscode.jdl] - Visual Studio Code

- **Jupyter** 583ms — Jupyter notebook support,... — Microsoft
- **Jupyter Keymap** — Jupyter keymaps for noteb... — Mic... — Reload Window
- **Jupyter Slide Show** — Jupyter Slide Show suppor... — Microsoft
- **Jupyter Cell Tags** — Jupyter Cell Tags support f... — Microsoft
- **Jupyter Notebook...** 12ms — Renderers for Jupyter Not... — Microsoft
- ~~**Jupyter (de...**~~ 805K ★ 3.5 — Data Science with Jupyter ... — Don Jayamanne — Install
- **Jupyter Pow...** 409K ★ 4.5 — Experimental features for ... — Microsoft — Install
- **VS Code Jup...** 632K ★ 3.5 — An easy to use extension f... — jithurjacob — Install
- **jupyter-note...** 137K ★ 1 — Runs jupyter notebooks in... — Sam Helms — Install
- **Jupyter Theme** 52K ★ 5 — A colour theme based aro... — SamCoding — Install
- **My Jupyter N...** 80K ★ 2.5 — My Jupyter Notebook Prev... — colinfang — Install
- **Jupyter TOC** 26K ★ 5 — Generate table of content... — xeladOm — Install

< Welcome

Get Started with Jupyter Notebooks

Your first steps to set up a Jupyter project with all the powerful tools and features that the Jupyter Extension has to offer!

○ **Create or open a Jupyter Notebook**

Right click in the file explorer and create a new file with an .ipynb extension. Or, open the Command Palette and run the command

`Create: New Jupyter Notebook.`

Create New Jupyter Notebook

If you have an existing project, you can also open a folder and/or clone a project from GitHub: clone a Git repository.

○ **Select a Jupyter kernel**

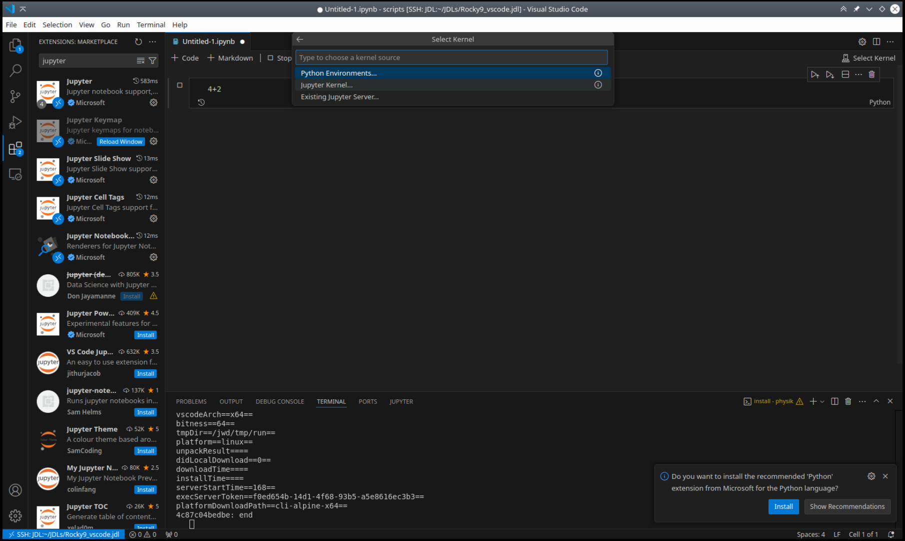
○ **Explore data and debug**

```
msg = "Welcome to Notebooks in VS Code!"
print(msg)
[1]
Welcome to Notebooks in VS Code!
```

```
vscodeArch==x64==
bitness==64==
tmpDir==/jwd/tmp/run==
platform==linux==
unpackResult====
didLocalDownload==0==
downloadTime====
installTime====
serverStartTime==168==
execServerToken==f0ed654b-14d1-4f68-93b5-a5e8616ec3b3==
platformDownloadPath==cli-alpine-x64==
4c87c04bedbe: end
```

Do you want to install the recommended 'Python' extension from Microsoft for the Python language?

Seeing it in action



● Untitled-1.ipynb - scripts [SSH: JDL:~/JDLs/Rocky9_vscode.jdl] - Visual Studio Code

Select Kernel

Type to choose a kernel source

- Python Environments...
- Jupyter Kernel...
- Existing Jupyter Server...

```
4+2
```

```
vscodeArch==x64==
bitness==64==
tmpDir==/jwd/tmp/run==
platform==linux==
unpackResult====
didLocalDownload==0==
downloadTime====
installTime====
serverStartTime==168==
execServerToken==f0ed654b-14d1-4f68-93b5-a5e8616ec3b3==
platformDownloadPath==cli-alpine-x64==
4c87c04bedbe: end
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File Edit Selection View Go Run Terminal Help
EXTENSIONS: MARKETPLACE
jupyter
Jupyter 583ms
Jupyter notebook support,...
Microsoft
Jupyter Keymap
Jupyter keymaps for noteb...
Mic... Reload Window
Jupyter Slide Show 13ms
Jupyter Slide Show suppor...
Microsoft
Jupyter Cell Tags 12ms
Jupyter Cell Tags support f...
Microsoft
Jupyter Notebook... 12ms
Renderers for Jupyter Not...
Microsoft
~~Jupyter (de...~~ 805K ★ 3.5
Data Science with Jupyter ...
Don Jayamanne Install
Jupyter Pow... 409K ★ 4.5
Experimental features for ...
Microsoft Install
VS Code Jup... 632K ★ 3.5
An easy to use extension f...
jithurjacob Install
jupyter-note... 137K ★ 1
Runs jupyter notebooks in...
Sam Helms Install
Jupyter Theme 52K ★ 5
A colour theme based aro...
SamCoding Install
My Jupyter N... 80K ★ 2.5
My Jupyter Notebook Prev...
colinfang Install
Jupyter TOC 26K ★ 5
Generate table of content...
xeladØm Install
Untitled-1.ipynb ●
+ Code + Markdown Stop
Select Kernel
Python
PROBLEMS OUTPUT DEBUG CONSOLE TERMINAL PORTS JUPYTER
install - physik
Install
Show Recommendations
SSH: JDL:~/JDLs/Rocky9_vscode.jdl
0 0 0
Spaces: 4 LF Cell 1 of 1

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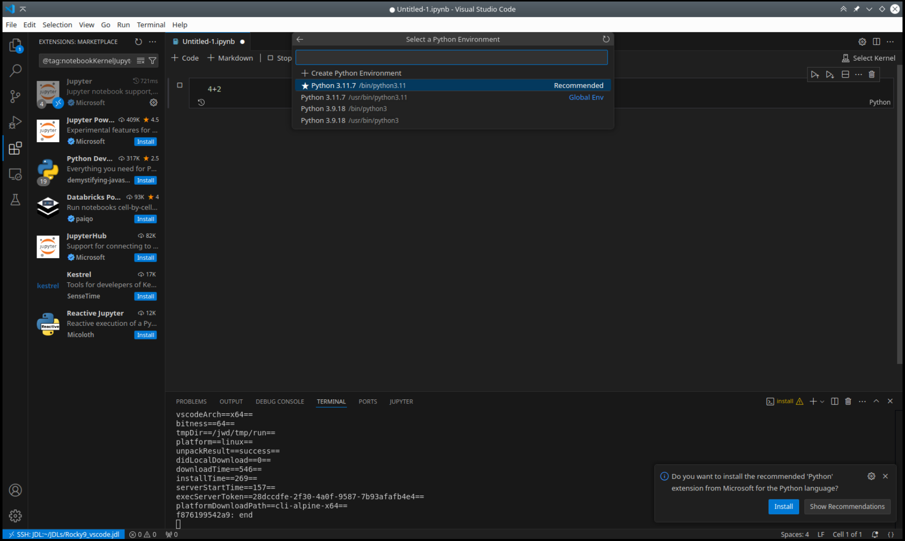
Seeing it in action



Select a Python Environment

+ Create Python Environment

★ Python 3.11.7 /bin/python3.11 Recommended

Python 3.11.7 /usr/bin/python3.11 Global Env

Python 3.9.18 /bin/python3

Python 3.9.18 /usr/bin/python3

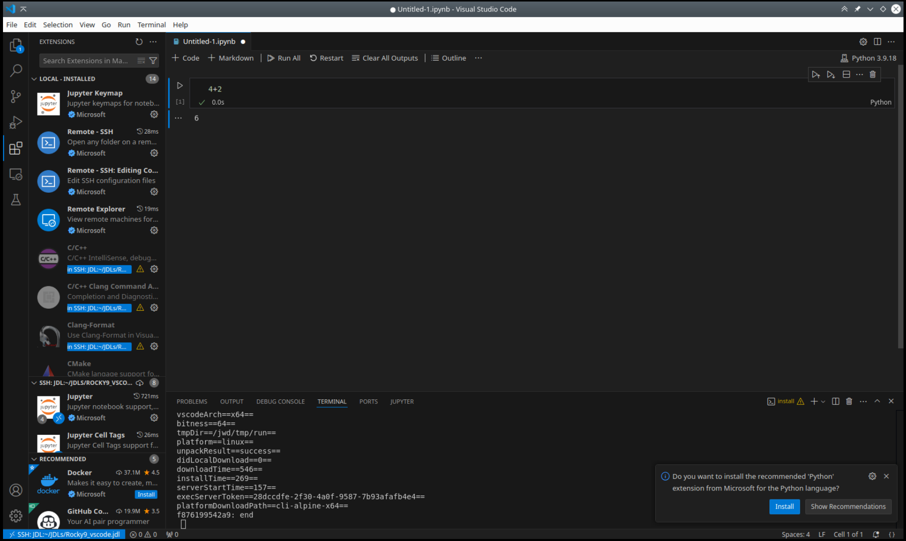
```
4+2
```

```
vscodeArch==x64==
bitness==64==
tmpDir==/jwd/tmp/run==
platform==linux==
unpackResult==success==
didLocalDownload==0==
downloadTime==546==
installTime==269==
serverStartTime==157==
execServerToken==28dccdfe-2f30-4a0f-9587-7b93afafb4e4==
platformDownloadPath==cli-alpine-x64==
f876199542a9: end
```

Do you want to install the recommended 'Python' extension from Microsoft for the Python language?

Install | Show Recommendations

Seeing it in action



● Untitled-1.ipynb - Visual Studio Code
File Edit Selection View Go Run Terminal Help
EXTENSIONS
Search Extensions in Ma...
LOCAL - INSTALLED 14
Jupyter Keymap
Jupyter keymaps for noteb...
Microsoft
Remote - SSH 28ms
Open any folder on a rem...
Microsoft
Remote - SSH: Editing Co...
Edit SSH configuration files
Microsoft
Remote Explorer 19ms
View remote machines for...
Microsoft
C/C++
C/C++ IntelliSense, debug...
in SSH: JDL:~/JDLs/R...
C/C++ Clang Command A...
Completion and Diagnosti...
in SSH: JDL:~/JDLs/R...
Clang-Format
Use Clang-Format in Visua...
in SSH: JDL:~/JDLs/R...
CMake
CMake langage support fo...
SSH: JDL:~/JDLS/ROCKY9_VSCO... 8
Jupyter 721ms
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Microsoft
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Jupyter Cell Tags support f...
RECOMMENDED 5
Docker 37.1M ★ 4.5
Makes it easy to create, m...
Microsoft
Install
GitHub Co... 19.9M ★ 3.5
Your AI pair programmer
Untitled-1.ipynb ●
+ Code + Markdown Run All Restart Clear All Outputs Outline ...
Python 3.9.18
[1]
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Python
PROBLEMS OUTPUT DEBUG CONSOLE TERMINAL PORTS JUPYTER
install
SSH: JDL:~/JDLs/Rocky9_vscode.jdl ⊗ 0 ⚠ 0 0
Spaces: 4 LF Cell 1 of 1

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```
vscodeArch==x64==
bitness==64==
tmpDir==/jwd/tmp/run==
platform==linux==
unpackResult==success==
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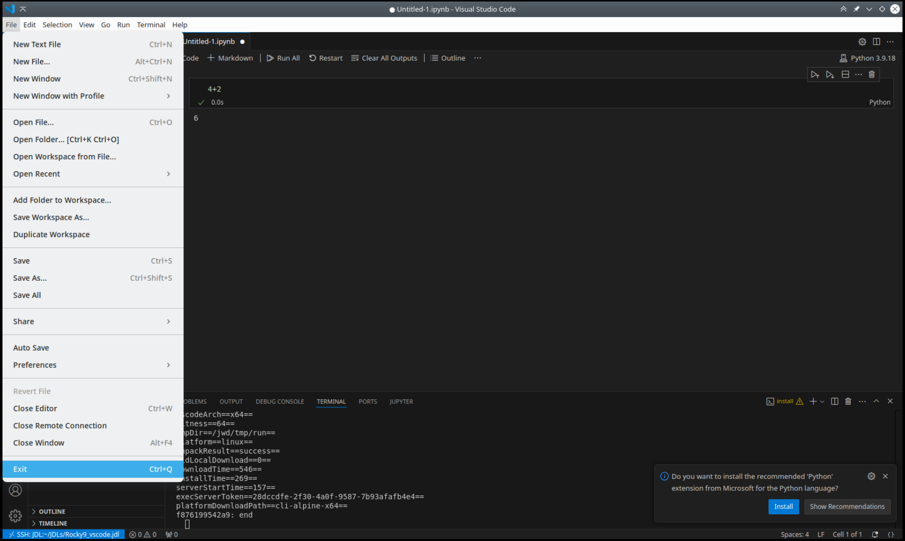
installTime==269==
serverStartTime==157==
execServerToken==28dccdfe-2f30-4a0f-9587-7b93afafb4e4==
platformDownloadPath==cli-alpine-x64==
f876199542a9: end
```

Do you want to install the recommended 'Python' extension from Microsoft for the Python language?

Install Show Recommendations

Seeing it in action



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```
scodeArch==x64==
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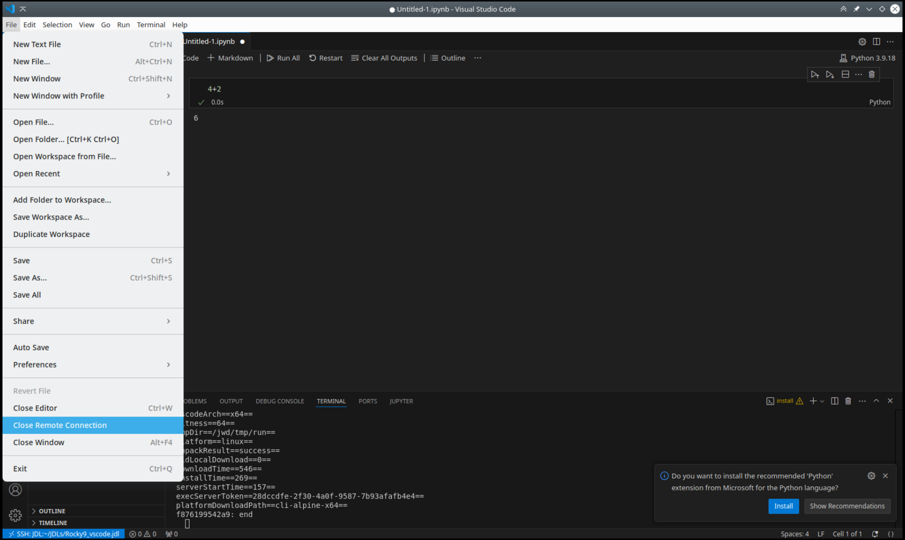
serverStartTime==157==
execServerToken==28dccdfe-2f30-4a0f-9587-7b93afafb4e4==
platformDownloadPath==cli-alpine-x64==
f876199542a9: end
```

Do you want to install the recommended 'Python' extension from Microsoft for the Python language?

Seeing it in action



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4+2
✓ 0.0s
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```
scodeArch==x64==
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npDir==/jwd/tmp/run==
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execServerToken==28dccdfe-2f30-4a0f-9587-7b93afafb4e4==
platformDownloadPath==cli-alpine-x64==
f876199542a9: end
```

Do you want to install the recommended 'Python' extension from Microsoft for the Python language?

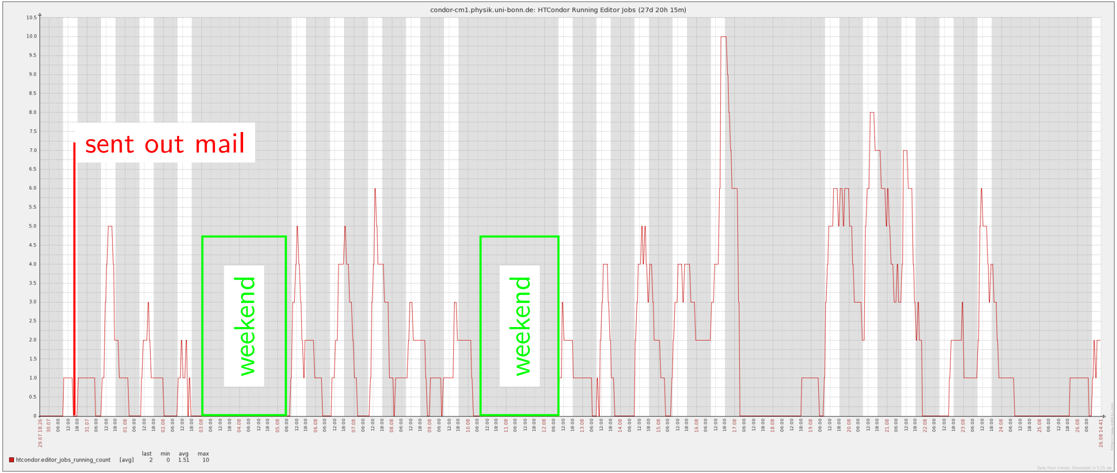
Known issues / caveats

- Since the jobs are not actual interactive jobs, they will not terminate when exiting VS Code
- Users can still place their code on the cluster's file system, causing degraded performance
- Users need to take active care of securing code changes, the job's HOME (i.e. working directory) is not persistent
- Custom `SSH` configs can cause issues, see this upstream issue
- Microsoft might push automatic updates resulting in the need for a different config
    - Already observed with an update on August 8th

Feedback and monitoring

- Quite positive feedback by users
- Some hiccups during first setups, resulted in extended FAQs / Troubleshooting notes
- Well received after rolling this out into production
- Jobs run within a new job flavor for easier monitoring
  - Easier monitoring with dedicated job flavor
  - Allows us to set some defaults and enforce limits for these jobs

Feedback and monitoring – Editing jobs

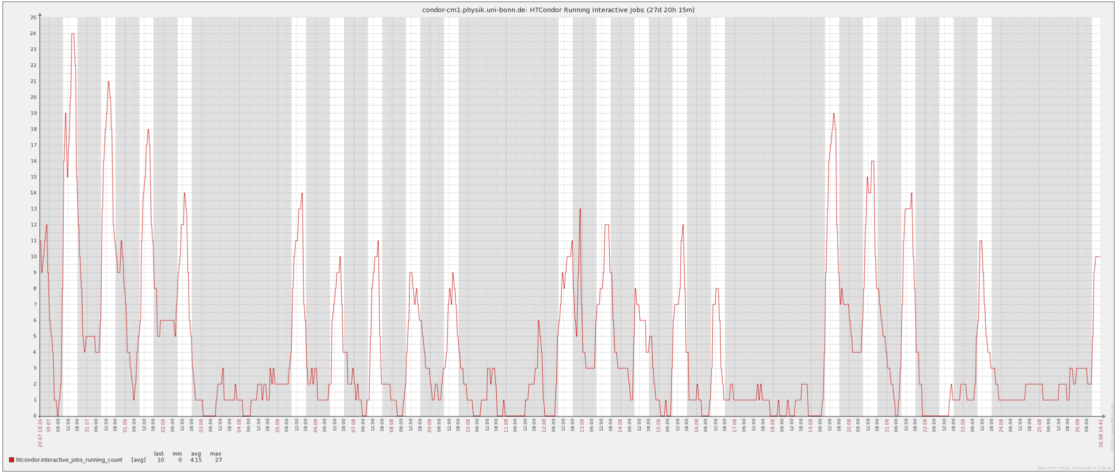


sent out mail

weekend

weekend

Feedback and monitoring – All interactive jobs



Conclusions

- ‘Interactive first’ approach works very well for us!
- Editing jobs via VS Code seem to be a nice addition to this approach
- You can make use of our VS Code integration in federated environments
- Code for custom `SSH` executable is publicly available on GitHub

Thank you!

Thank you

for your attention!

☕