

Introduction to Visual Studio Code



<https://github.com/Whitford/ctbp-techtalks>

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VS Code - Visual Studio Code

Visual Studio Code is a source code editor that can be used with a variety of programming languages, including C, C#, C++, Fortran, Go, Java, JavaScript, Node.js, Python, Rust, Julia, and more.

- No. 1 – Dev tool since 2018 – Stack Overflow
- Open-Source Software



Microsoft

VS Code – Pros vs Cons

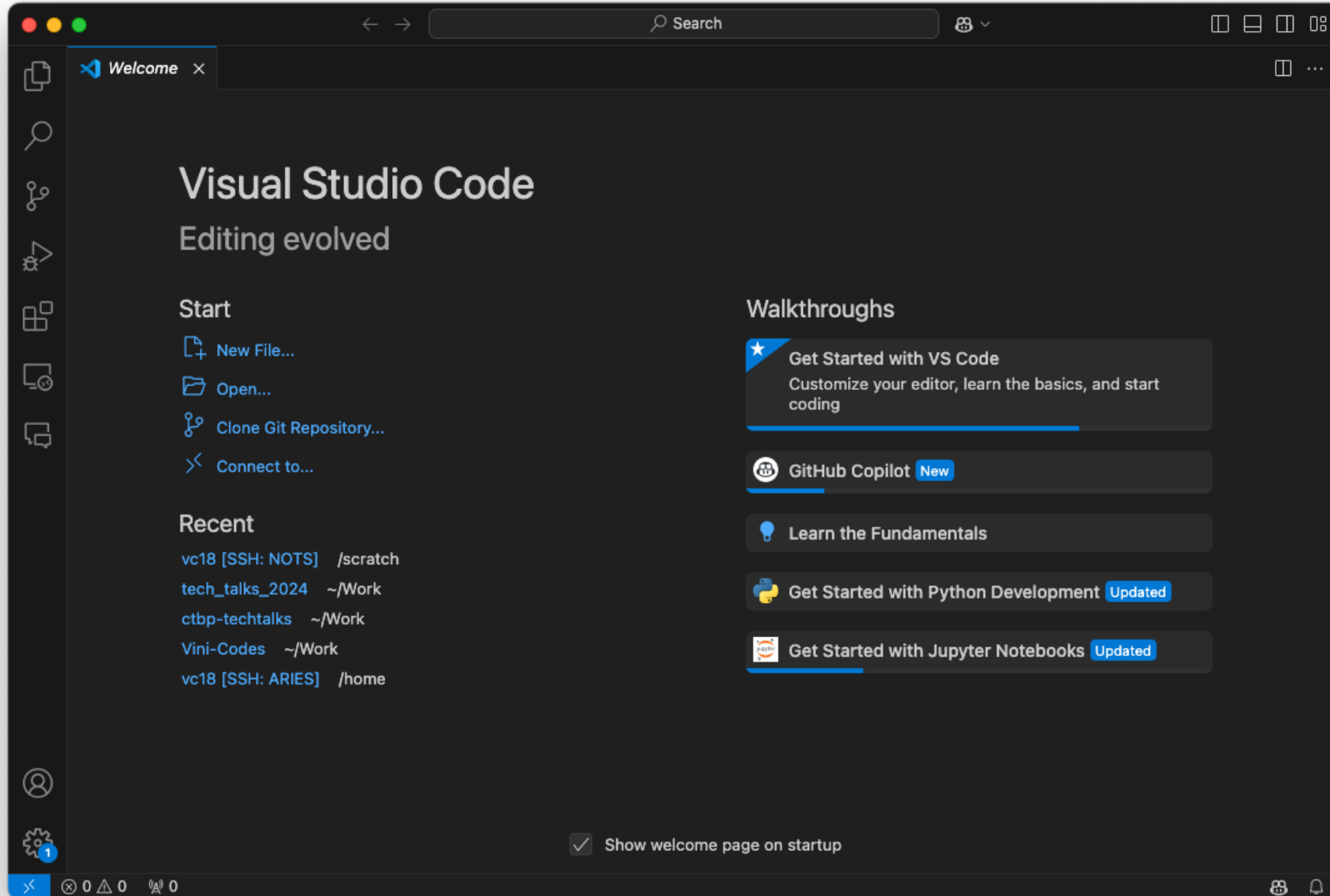
PROS

- Lightweight – Multi-Platform
- Extensions – Customizable
 - Integrated with Git
 - Remote access – SSH
 - Built-in Terminal
- Jupyter Notebook

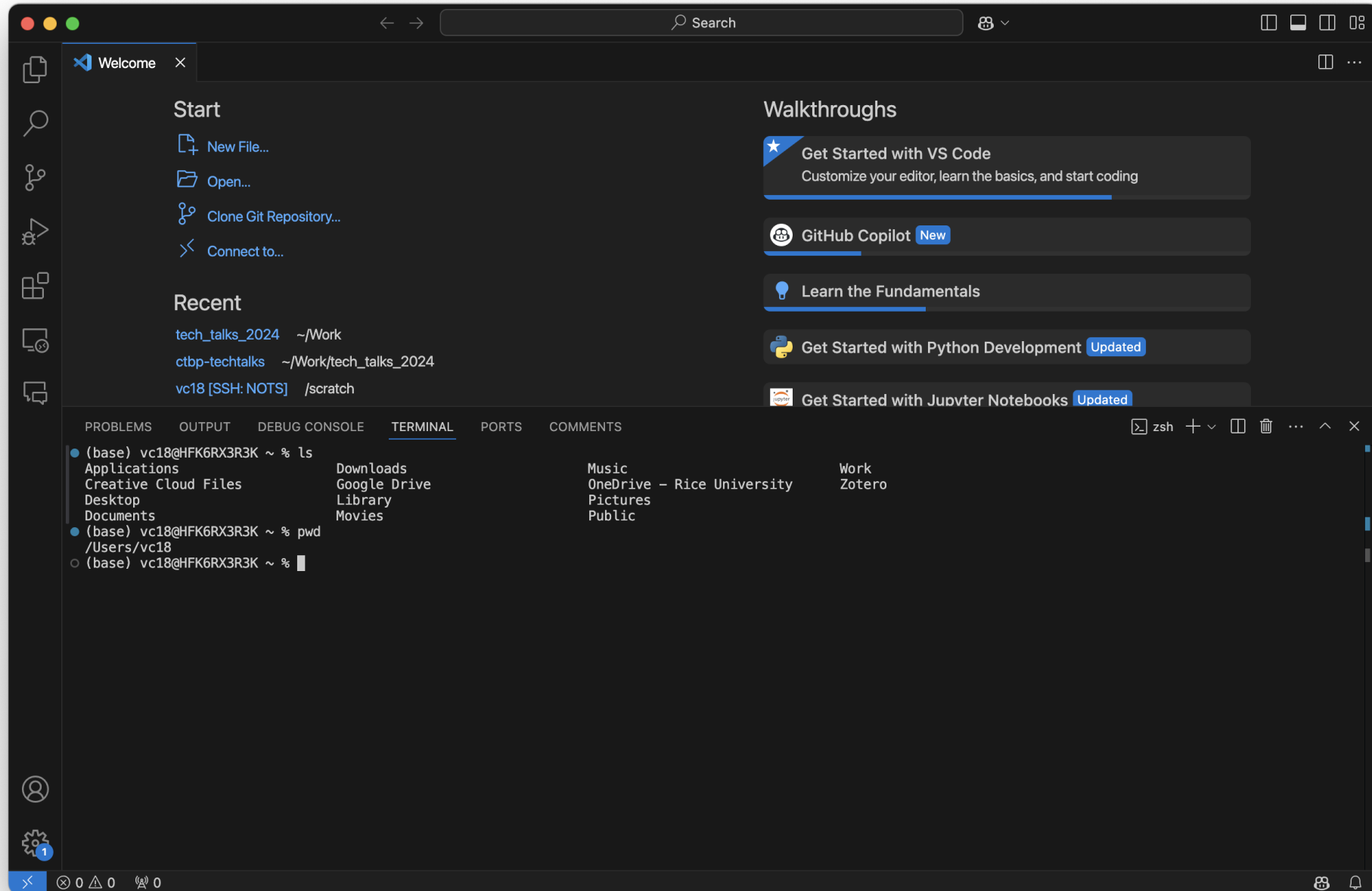
CONS

- Learning Curve
- Dependency on Extensions
- Not a full IDE (Integrated Development Environment)

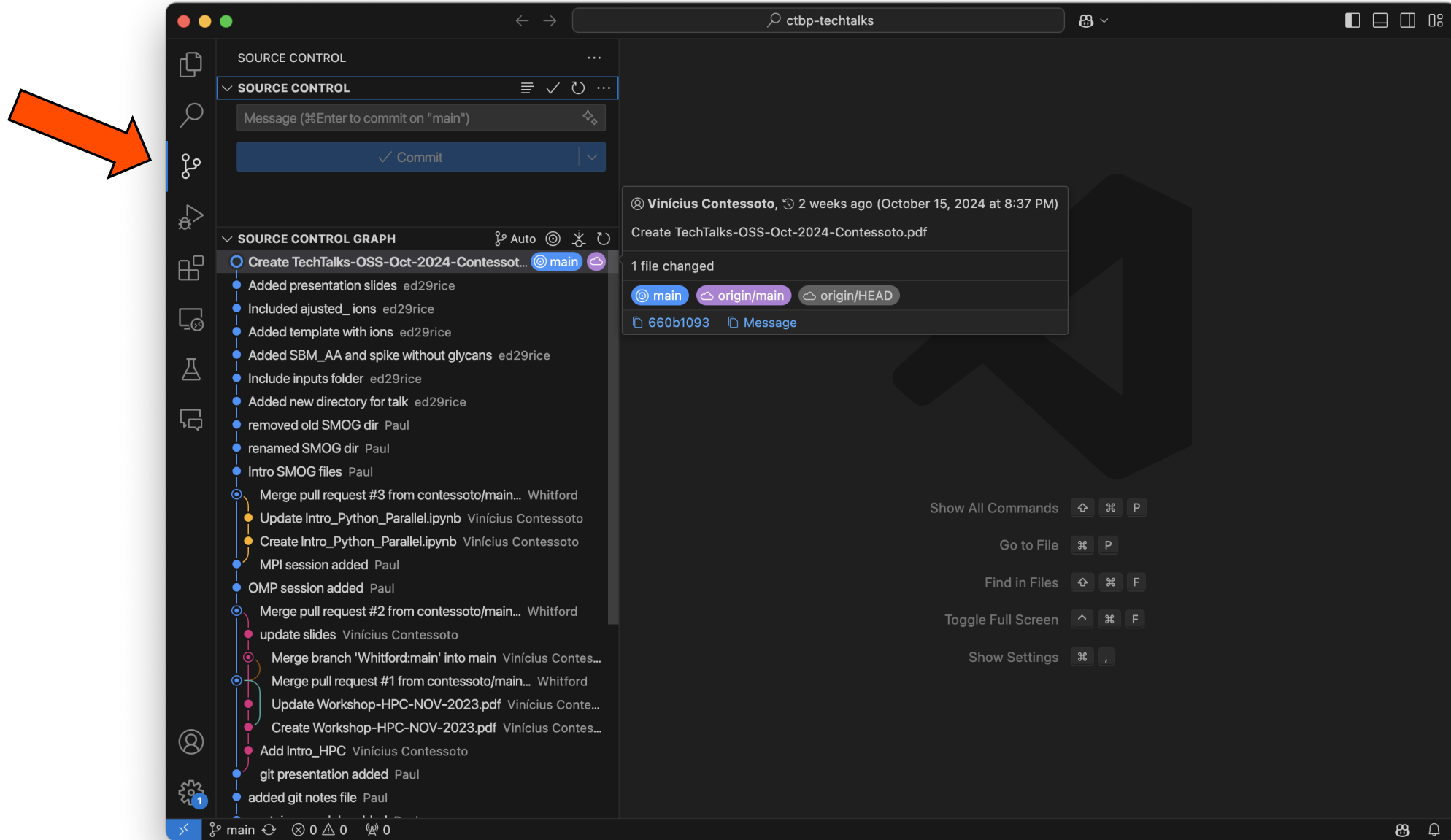
Interface



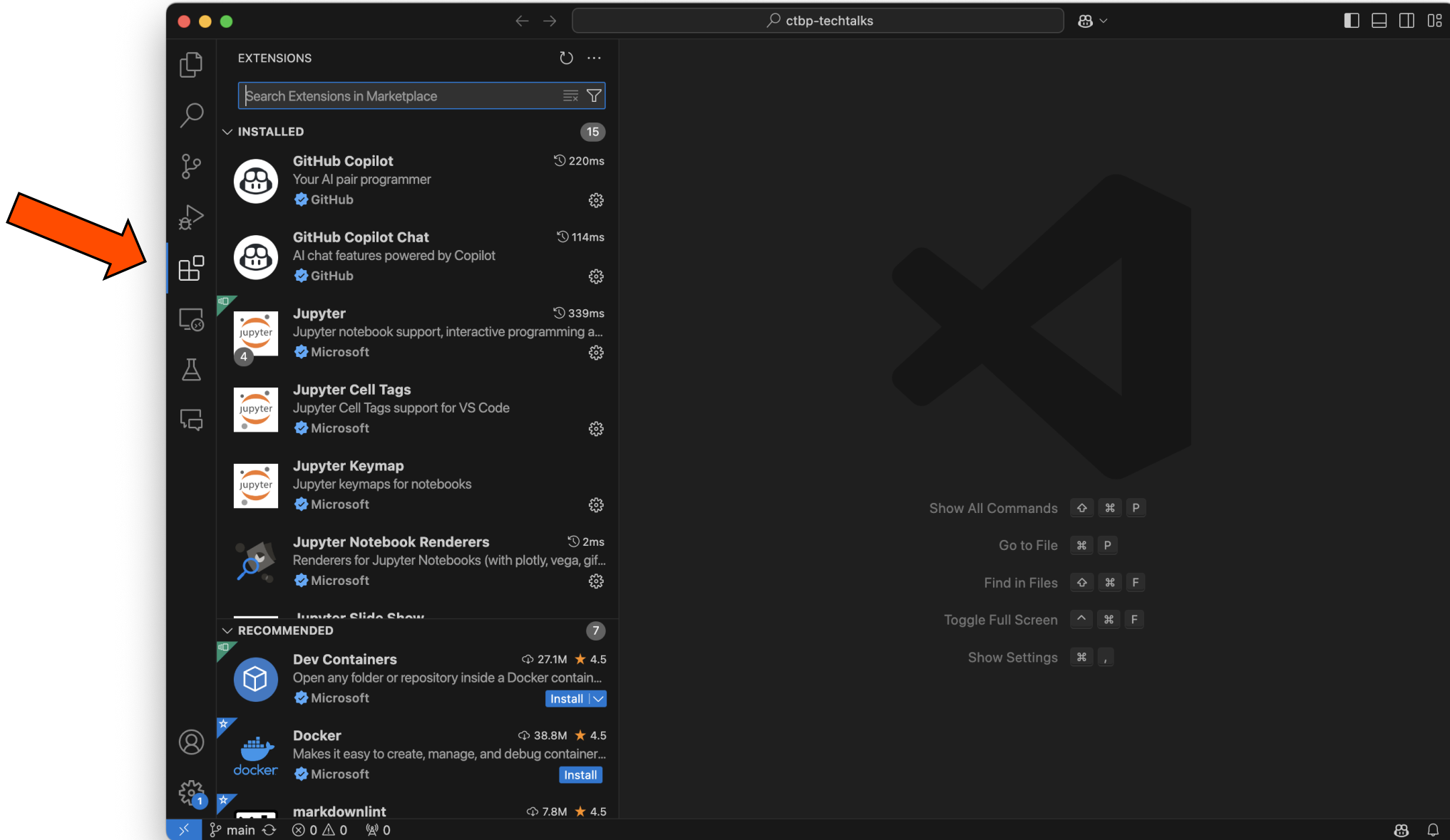
Terminal



Git



Extensions



Protein Viewer

The screenshot displays the Protein Viewer application interface. The central window shows a 3D ribbon model of a protein structure, colored with a green-to-yellow gradient. The interface includes a top navigation bar with a search bar and a user profile icon. On the left, a 'State Tree' panel lists the hierarchy: 2A3D 1 model, Model 1, Assembly 1 (1140 elements), Polymer (1140 elements), and Cartoon. Below this is a 'Measurements' section. The top right panel shows the 'Sequence of 2A3D | SOLUTION STRUCTURE O...' with a sequence: MGSWAEFKQRLAAIKTRLQALGGSEAEIAAFEKEIAAFESLQAYKGKGNPEVEALRKEAAAI⁶¹DELQAYRHN⁷¹. The right sidebar contains 'Structure Tools' with sections for Structure, Measurements, Quick Styles, Components, Assembly Symmetry, Export Models, Export Animation, and Export Geometry. The bottom status bar shows a timeline of updates: 9:13:23 Updated Cartoon in 16ms., 9:13:29 Updated Cartoon in 15ms., and 9:13:36 Updated Cartoon in 14ms.

Protein Viewer - X

State Tree

- 2A3D 1 model
- Model 1
- Assembly 1 1140 elements
- Polymer 1140 elements
- Cartoon
- Update 3D Representation
- Apply Action
- Measurements

Sequence of 2A3D | SOLUTION STRUCTURE O... Chain 1: PROTEIN (... A

1 11 21 31 41 51 61 71
MGSWAEFKQRLAAIKTRLQALGGSEAEIAAFEKEIAAFESLQAYKGKGNPEVEALRKEAAAI⁶¹DELQAYRHN⁷¹

Structure Tools

Structure

2A3D | SOLUTION STRUCTURE O...

Type	Assembly
Asm Id	1: Author Defined Asse...
Dynamic Bonds	X Off

Nothing Focused

Measurements

+ Add

Quick Styles

Default Stylized Illustrative

Components 2A3D

Preset + Add

Polymer Cartoon

Assembly Symmetry 2A3D

✓ Enable

Export Models

Export Animation

Export Geometry

PROTEIN (DE NOVO THREE-HELIX BUNDLE)
2A3D | Model 1 | Instance ASM_1 | A | ARG 64

9:13:23 Updated Cartoon in 16ms.
9:13:29 Updated Cartoon in 15ms.
9:13:36 Updated Cartoon in 14ms.

main 0 0 0

GitHub Copilot



The screenshot displays a Jupyter Notebook environment with the following sections:

- Import Required Libraries**
Import the necessary libraries, including Biopython and NumPy.
Code:

```
# Import the necessary libraries, including Biopython and NumPy
from Bio.PDB import PDBList, PDBParser
import numpy as np
```
- Fetch Protein Data from PDB**
Use Biopython to fetch the PDB file for the protein with PDB ID 2a3d.
Code:

```
# Fetch Protein Data from PDB

# Create a PDBList object to fetch the PDB file
pdbl = PDBList()

# Fetch the PDB file for the protein with PDB ID 2a3d
pdb_id = "2a3d"
pdb_file = pdbl.retrieve_pdb_file(pdb_id, file_format="pdb")

# Parse the PDB file to get the structure
parser = PDBParser()
structure = parser.get_structure(pdb_id, pdb_file)

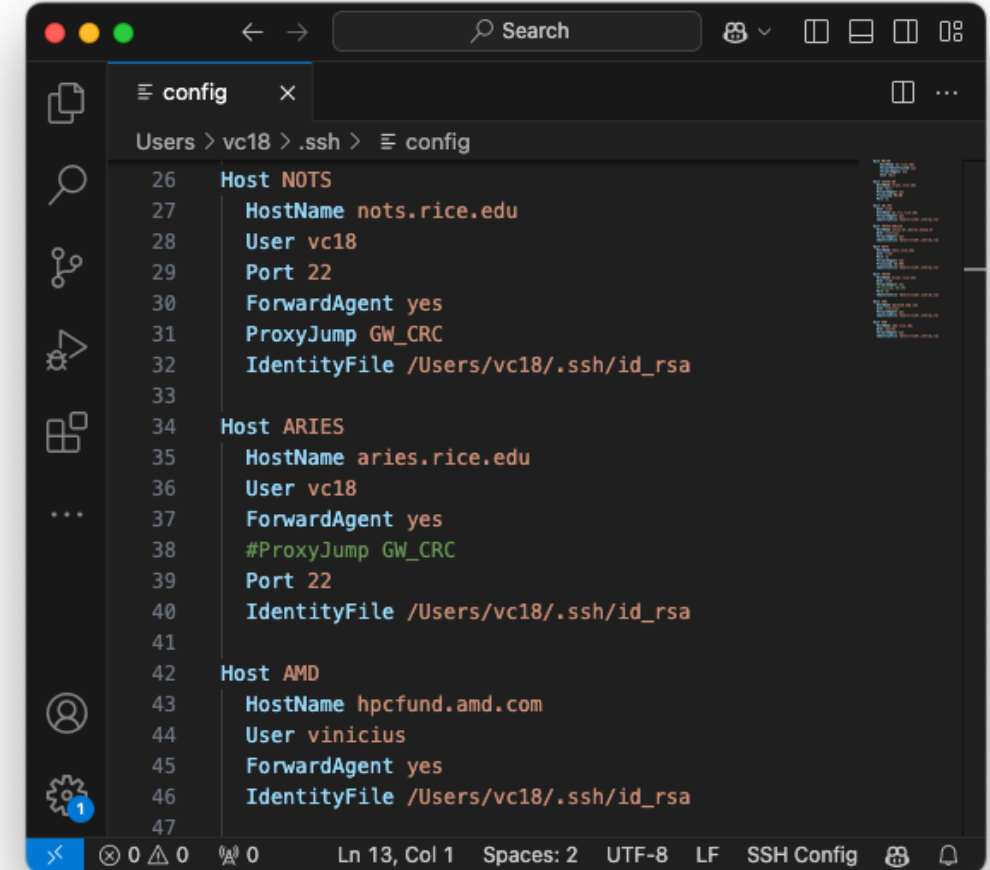
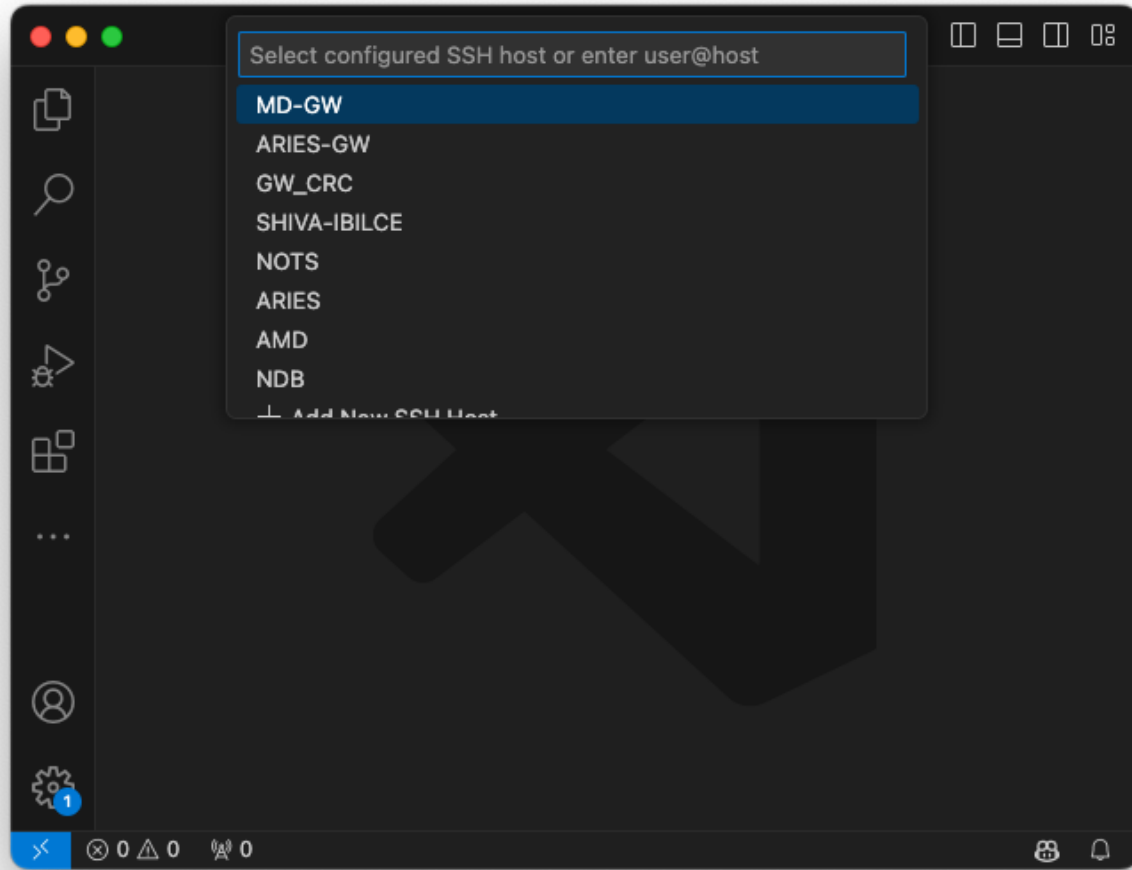
# Print the structure to verify
print(structure)
```
- Parse PDB File**

The right-hand panel contains a chat window with the user's request: "I need to create a jupyter notebook for calculating the radius of gyration of all c-alpha from my protein with pdb id 2a3d. i need to fetch this data from the PDB. give me the code and the notebook with all functions very well detailed." Below the chat is a table of contents for the notebook:

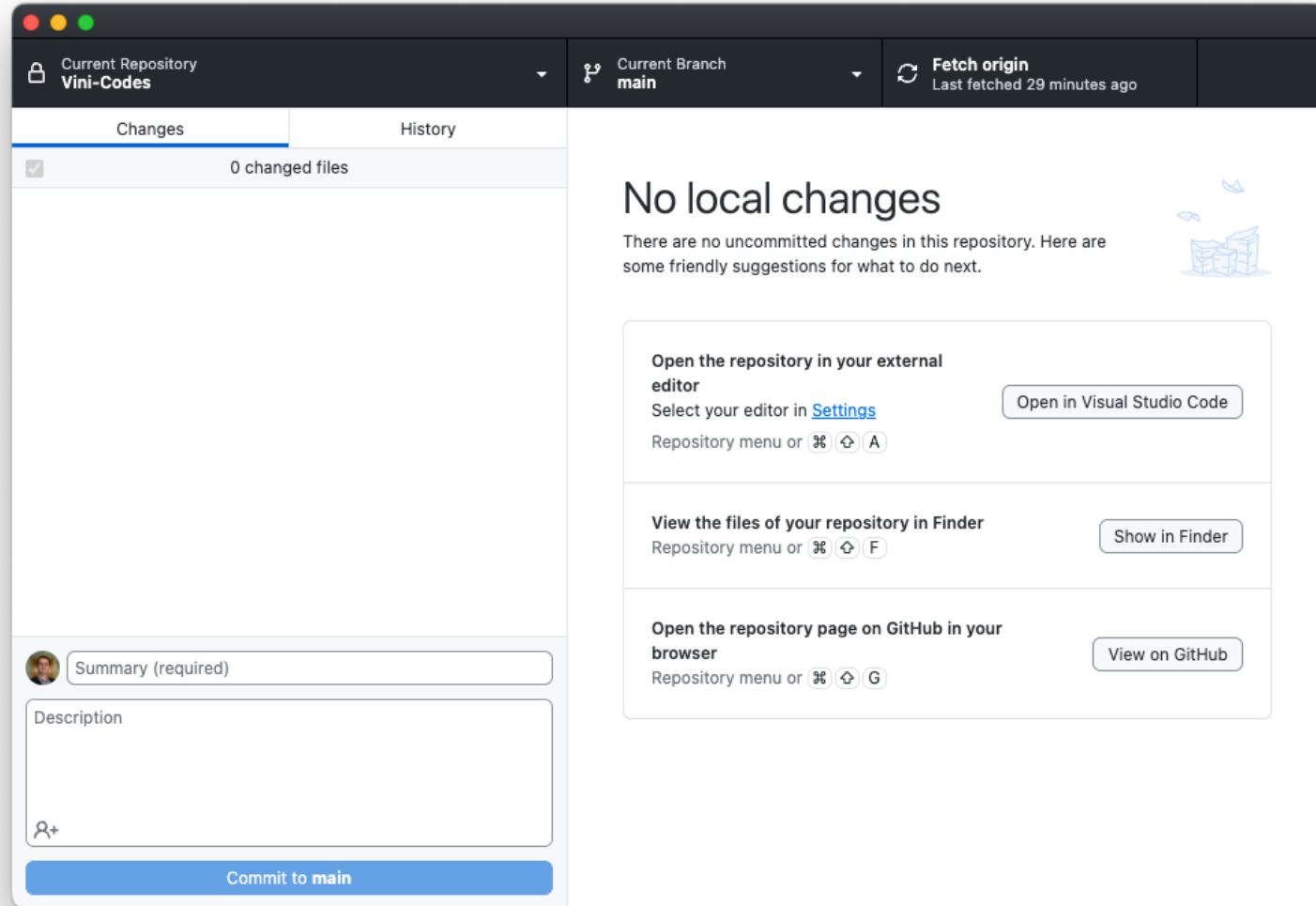
- Import Required Libraries
- Fetch Protein Data from PDB
- Parse PDB File
- Extract C-alpha Atoms
- Calculate Radius of Gyration

A "Create Notebook" button is visible below the table of contents.

Remote SSH



GitHub Desktop



<https://github.com/Whitford/ctbp-techtalks>

CTBP – Resources & Useful links

- <https://github.com/Whitford/ctbp-techtalks> (Tech Talks Slides and Files)
- <https://ctbp.rice.edu/ctbp-tech-talks> (Tech Talks Schedule)
- <https://kb.rice.edu/page.php?id=108237> (NOTS)
- <https://wiki.rice.edu/confluence/display/CTBP/CTBP+Computing+Activities> (CTBP)
- <https://code.visualstudio.com> (VS Code)
- <https://github.com/apps/desktop> (GitHub Desktop)