

A reproducible thesis

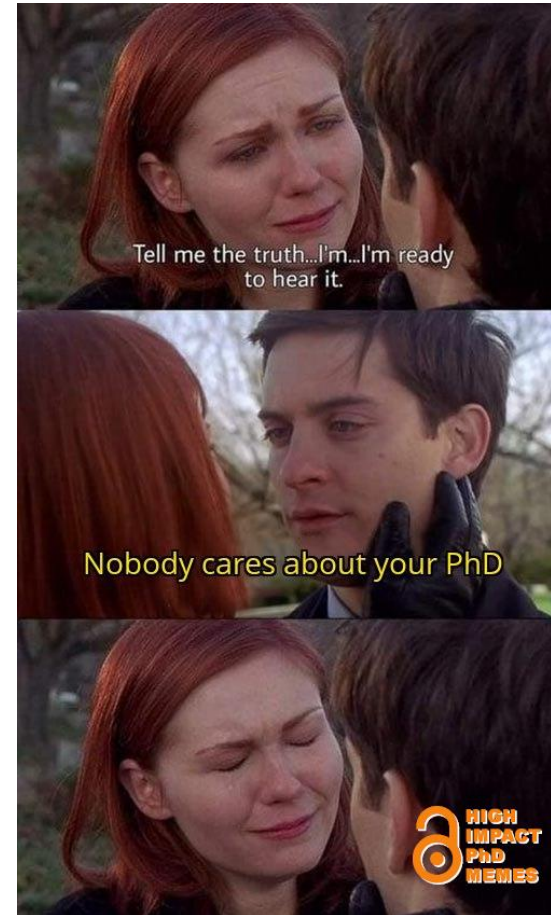
Writing code and reports in one go with Snakemake and R Markdown

Expectations vs. reality

Expectations vs. reality



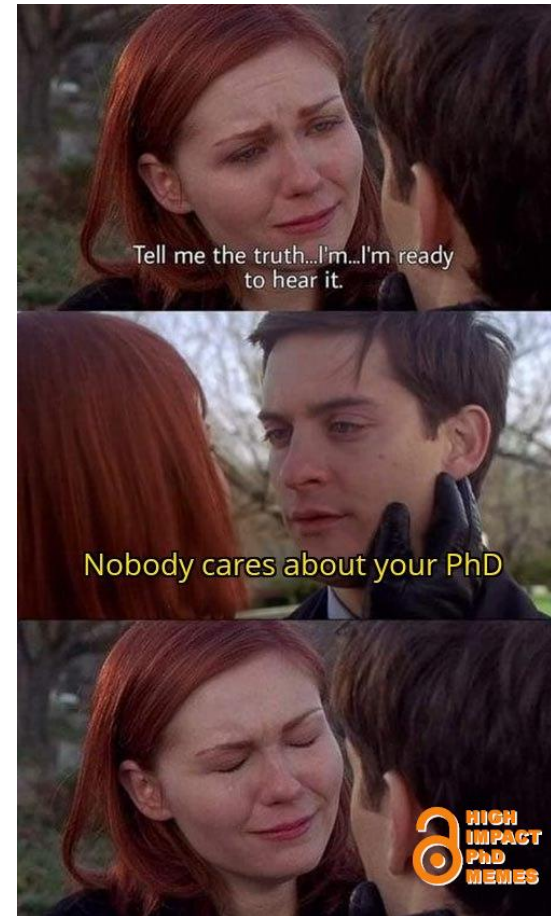
Expectations vs. reality



Expectations vs. reality



Why is the cat sad?

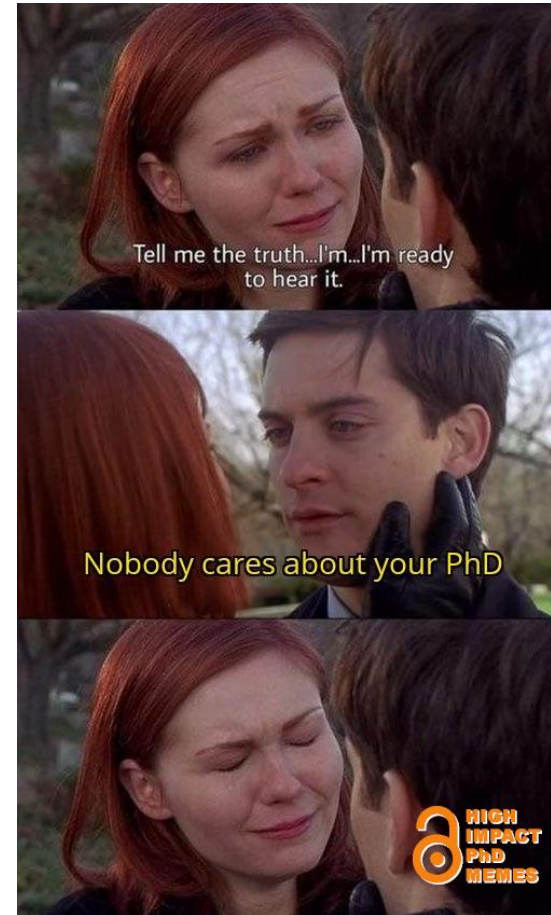


Expectations vs. reality



Why is the cat sad?

- They spent ages doing analysis
- They spent little time writing

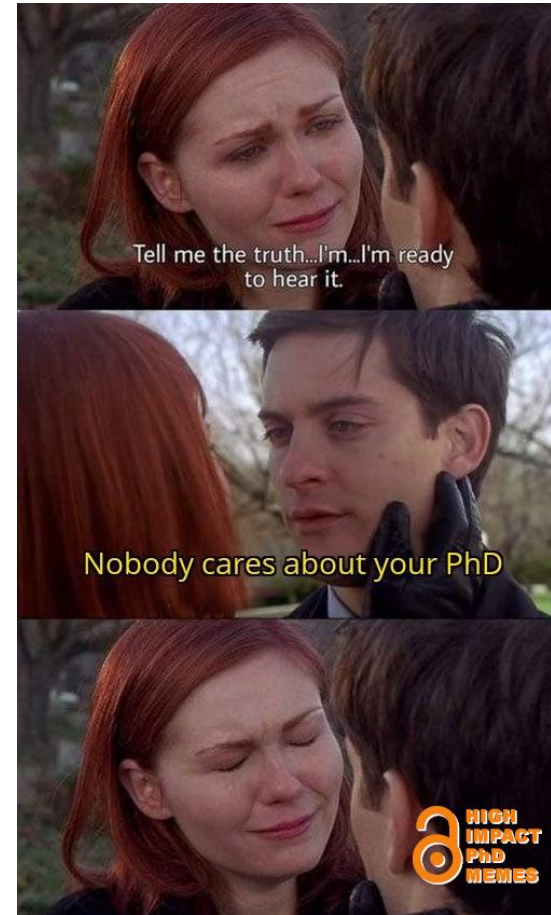


Expectations vs. reality



Why is the cat sad?

- They spent ages doing analysis
- They spent little time writing



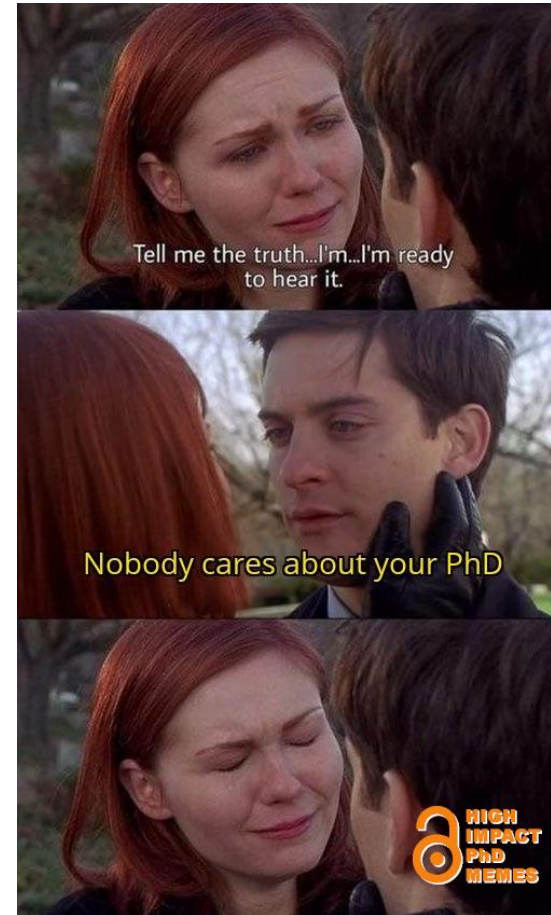
Why is the woman regretful?

Expectations vs. reality



Why is the cat sad?

- They spent ages doing analysis
- They spent little time writing



Why is the woman regretful?

- Her work is not reproducible
- Her work is not adaptable
- Her work is not transparent

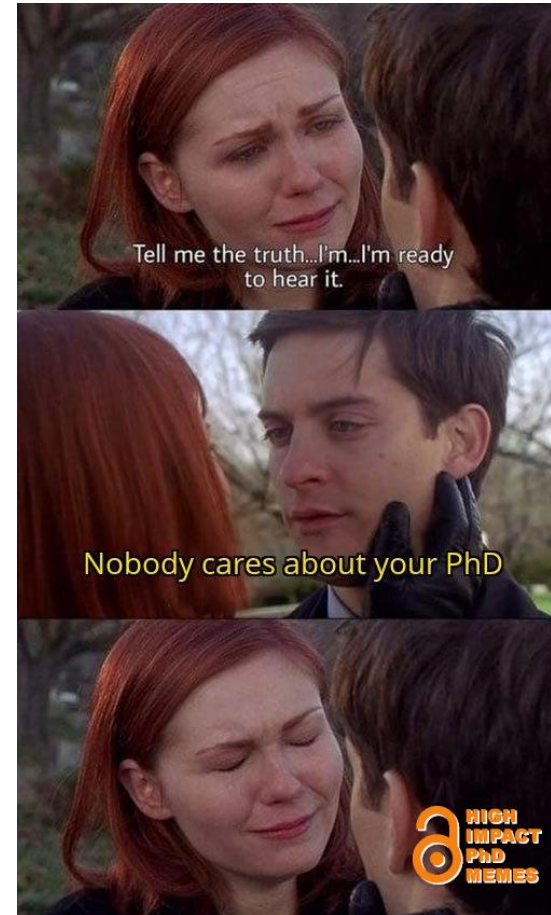
Expectations vs. reality



One simple trick...

Why is the cat sad?

- They spent ages doing analysis
- They spent little time writing



Why is the woman regretful?

- Her work is not reproducible
- Her work is not adaptable
- Her work is not transparent

The solution: a reproducible workflow



The solution: a reproducible workflow

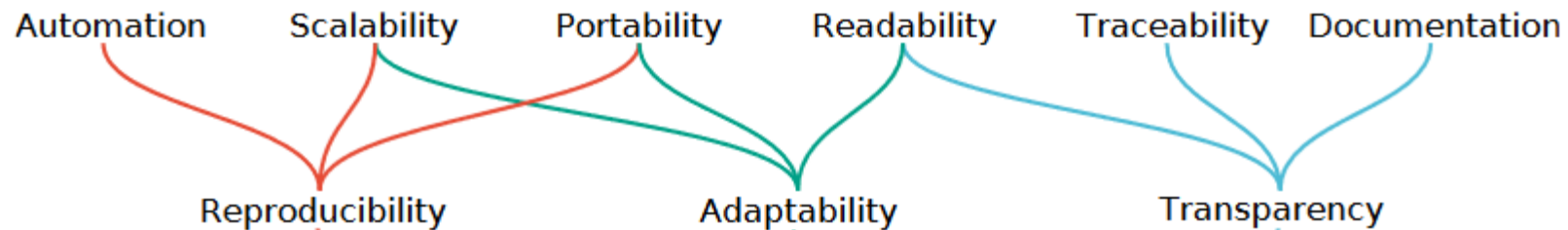


Reproducibility

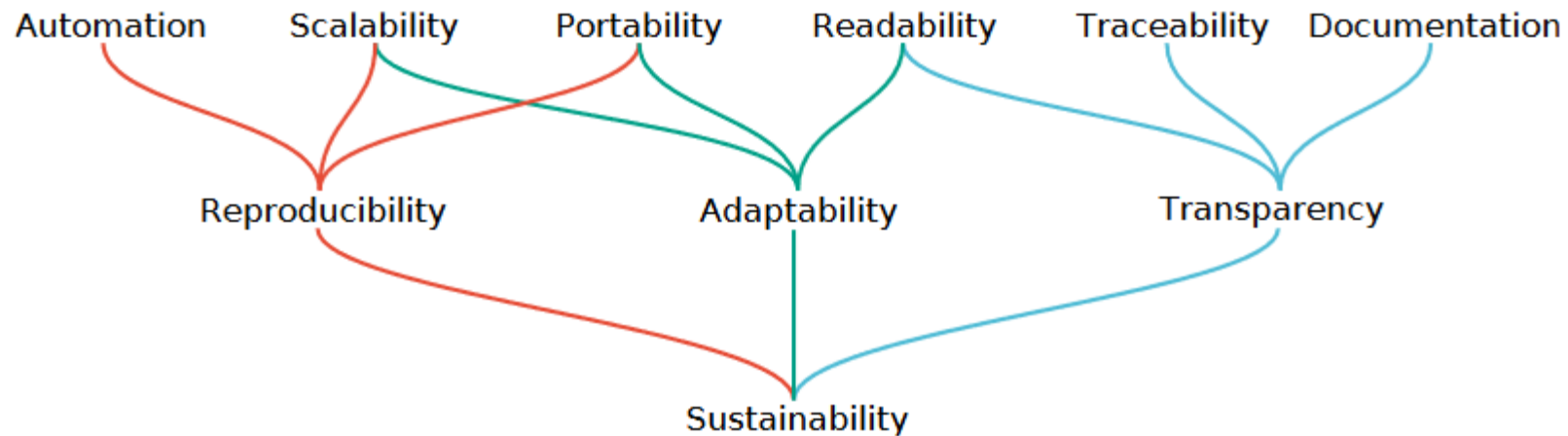
Adaptability

Transparency

The solution: a reproducible workflow



The solution: a reproducible workflow



A flavour of snakemake

A flavour of snakemake

Rule: assemble sandwich

Output: **sandwich**

Input:

- **sliced_ingredient**
- **sauce**

A flavour of snakemake

Rule: slice ingredient
Output: **sliced_ingredient**
Input: **ingredient**

Rule: assemble sandwich
Output: **sandwich**
Input:

- **sliced_ingredient**
- **sauce**

A flavour of snakemake

Rule: slice ingredient
Output: **sliced_ingredient**
Input: **ingredient**

Rule: make sauce
Output: **sauce**
Input: **sauce_ingredients**

Rule: assemble sandwich
Output: **sandwich**
Input:

- **sliced_ingredient**
- **sauce**

A flavour of snakemake

○○○

```
rule slice ingredient:  
    output: "sliced_{ingredient}"  
    input: "{ingredient}"  
    shell:  
        "slice {input} > {output}"
```

Rule: slice ingredient
Output: **sliced_ingredient**
Input: **ingredient**

Rule: make sauce
Output: **sauce**
Input: **sauce_ingredients**

Rule: assemble sandwich
Output: **sandwich**
Input:
• **sliced_ingredient**
• **sauce**

Snakemake-ing a sandwich

Snakemake-ing a sandwich

Rule: assemble sandwich

Output: **italian_sandwich**

Input:

- **sliced_tomatoes**
- **sliced_mozzarella**
- **sliced_panini**
- **pesto_sauce**

Snakemake-ing a sandwich

Rule: assemble sandwich

Output: **italian_sandwich**

Input:

- **sliced_tomatoes**
- **sliced_mozzarella**
- **sliced_panini**
- **pesto_sauce**

○ ○ ○

```
Snakemake italian_sandwich
```

Snakemake-ing a sandwich

Rule: slice ingredient

Output: **sliced_tomatoes**

Input:

- **tomatoes**

Rule: assemble sandwich

Output: **italian_sandwich**

Input:

- **sliced_tomatoes**
- **sliced_mozzarella**
- **sliced_panini**
- **pesto_sauce**

○ ○ ○

```
Snakemake italian_sandwich
```

Snakemake-ing a sandwich

Rule: slice ingredient

Output: **sliced_tomatoes**

Input:

- **tomatoes**

Rule: slice ingredient

Output: **sliced_mozzarella**

Input:

- **mozzarella**

Rule: assemble sandwich

Output: **italian_sandwich**

Input:

- **sliced_tomatoes**
- **sliced_mozzarella**
- **sliced_panini**
- **pesto_sauce**

○ ○ ○

```
Snakemake italian_sandwich
```

Snakemake-ing a sandwich

Rule: slice ingredient
Output: **sliced_tomatoes**
Input:
• **tomatoes**

Rule: slice ingredient
Output: **sliced_mozzarella**
Input:
• **mozzarella**

Rule: slice ingredient
Output: **sliced_panini**
Input:
• **panini**

Rule: assemble sandwich
Output: **italian_sandwich**
Input:
• **sliced_tomatoes**
• **sliced_mozzarella**
• **sliced_panini**
• **pesto_sauce**

○ ○ ○

```
Snakemake italian_sandwich
```

Snakemake-ing a sandwich

Rule: slice ingredient
Output: **sliced_tomatoes**
Input:
• **tomatoes**

Rule: slice ingredient
Output: **sliced_mozzarella**
Input:
• **mozzarella**

Rule: slice ingredient
Output: **sliced_panini**
Input:
• **panini**

Rule: make sauce
Output: **pesto_sauce**
Input:
• **pesto_sauce_ingredients**

Rule: assemble sandwich
Output: **italian_sandwich**
Input:
• **sliced_tomatoes**
• **sliced_mozzarella**
• **sliced_panini**
• **pesto_sauce**

○ ○ ○

```
Snakemake italian_sandwich
```


Snakemake-ing a sandwich

Rule: slice ingredient
Output: **sliced_tomatoes**
Input:
• **tomatoes**

Rule: slice ingredient
Output: **sliced_mozzarella**
Input:
• **mozzarella**

Rule: slice ingredient
Output: **sliced_panini**
Input:
• **panini**

Rule: make sauce
Output: **pesto_sauce**
Input:
• **pesto_sauce_ingredients**

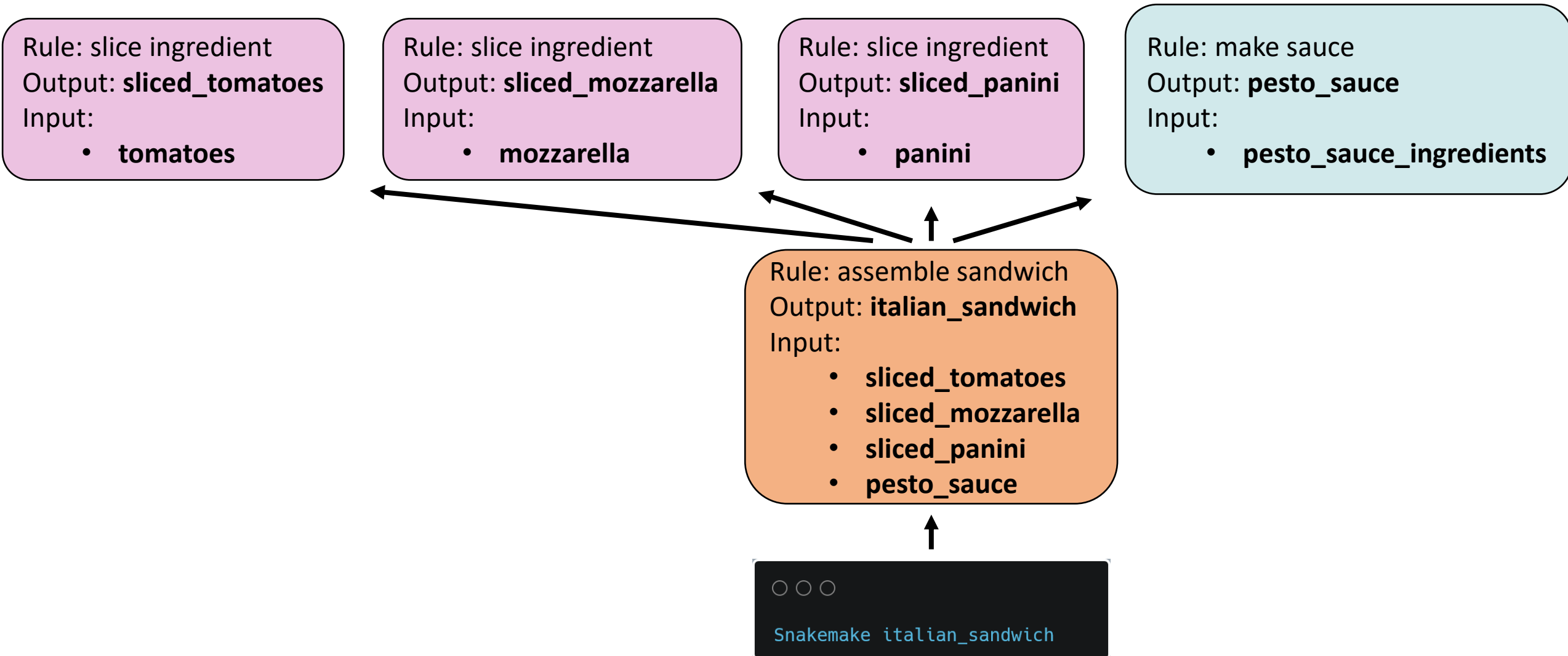
Rule: assemble sandwich
Output: **italian_sandwich**
Input:
• **sliced_tomatoes**
• **sliced_mozzarella**
• **sliced_panini**
• **pesto_sauce**



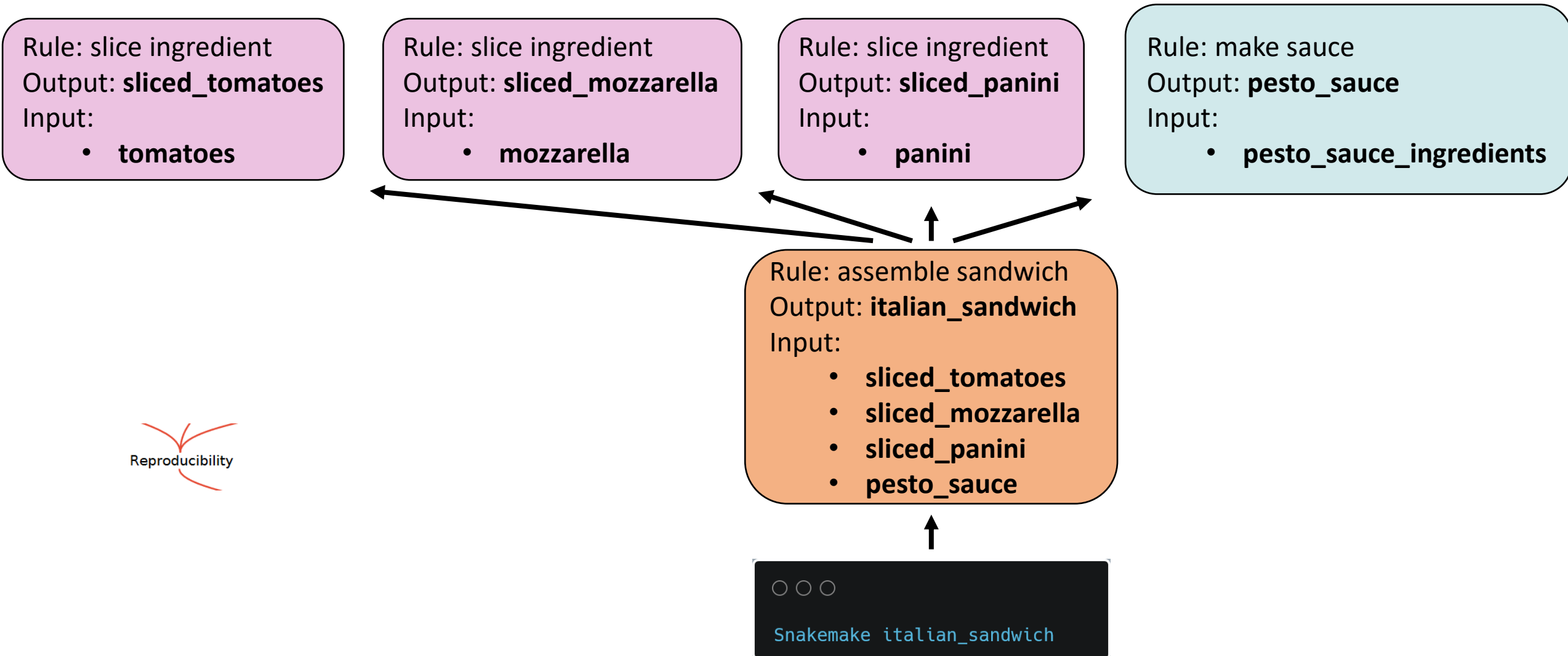
○ ○ ○

```
Snakemake italian_sandwich
```

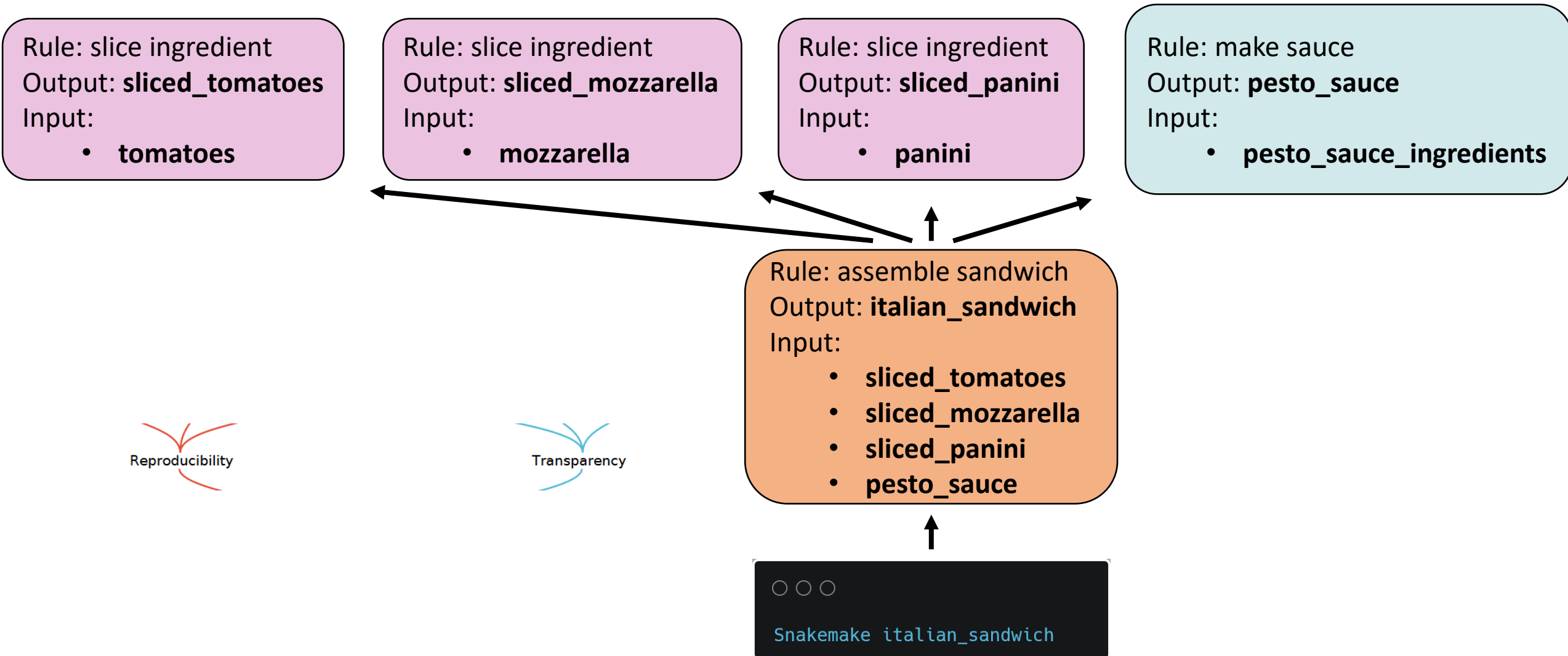
Snakemake-ing a sandwich



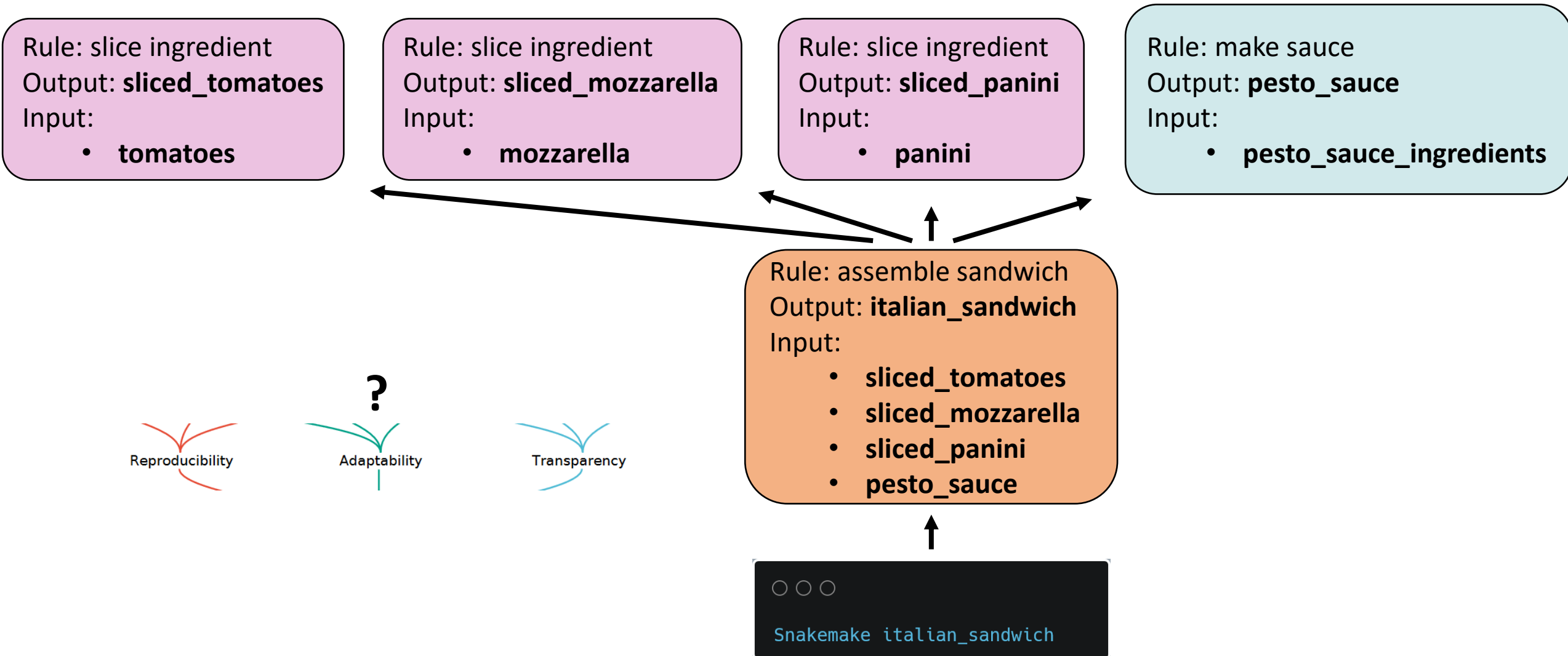
Snakemake-ing a sandwich



Snakemake-ing a sandwich



Snakemake-ing a sandwich



My Middle Eastern friend doesn't like Italian sandwiches...

My Middle Eastern friend doesn't like Italian sandwiches...

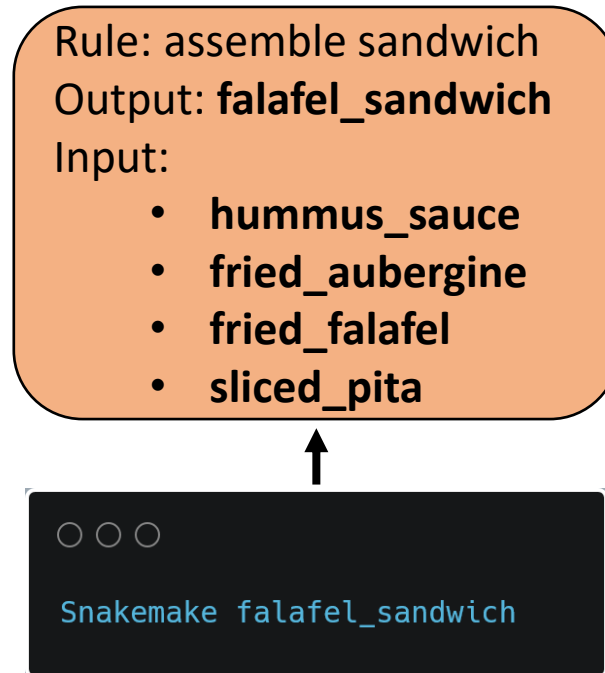
Rule: assemble sandwich

Output: **falafel_sandwich**

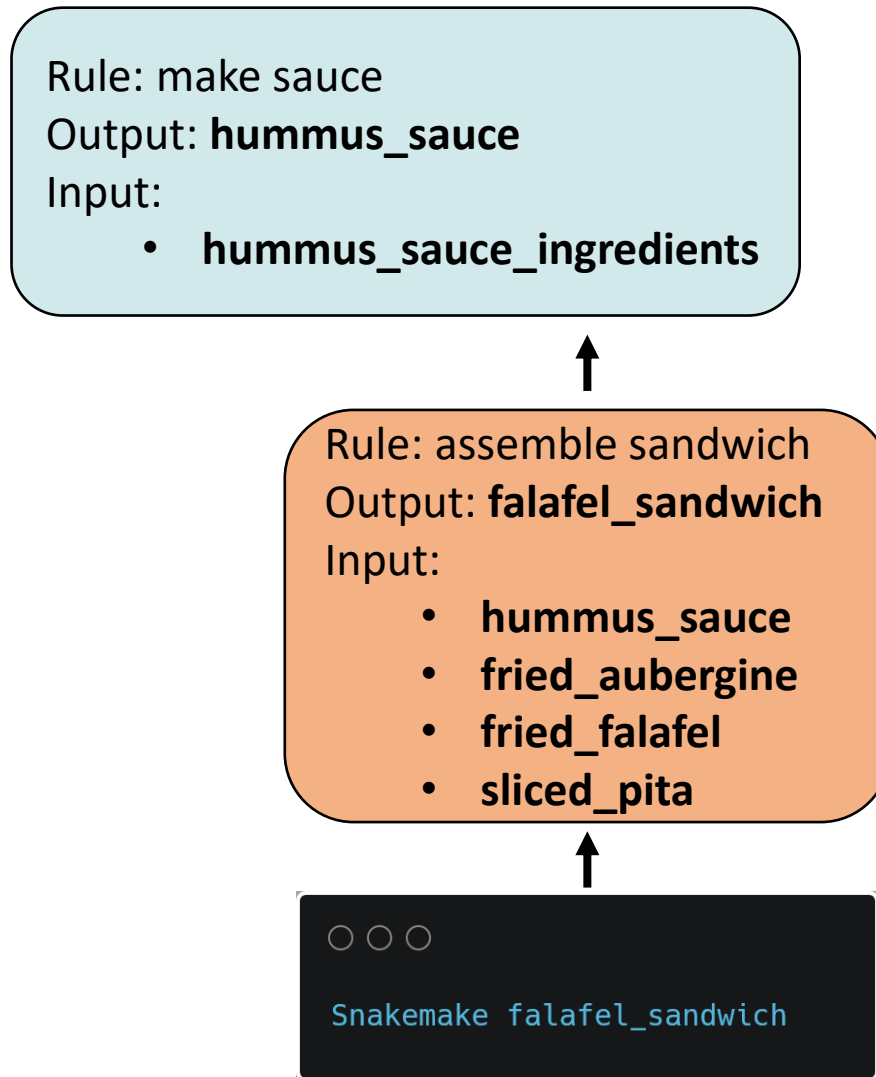
Input:

- hummus_sauce
- fried_aubergine
- fried_falafel
- sliced_pita

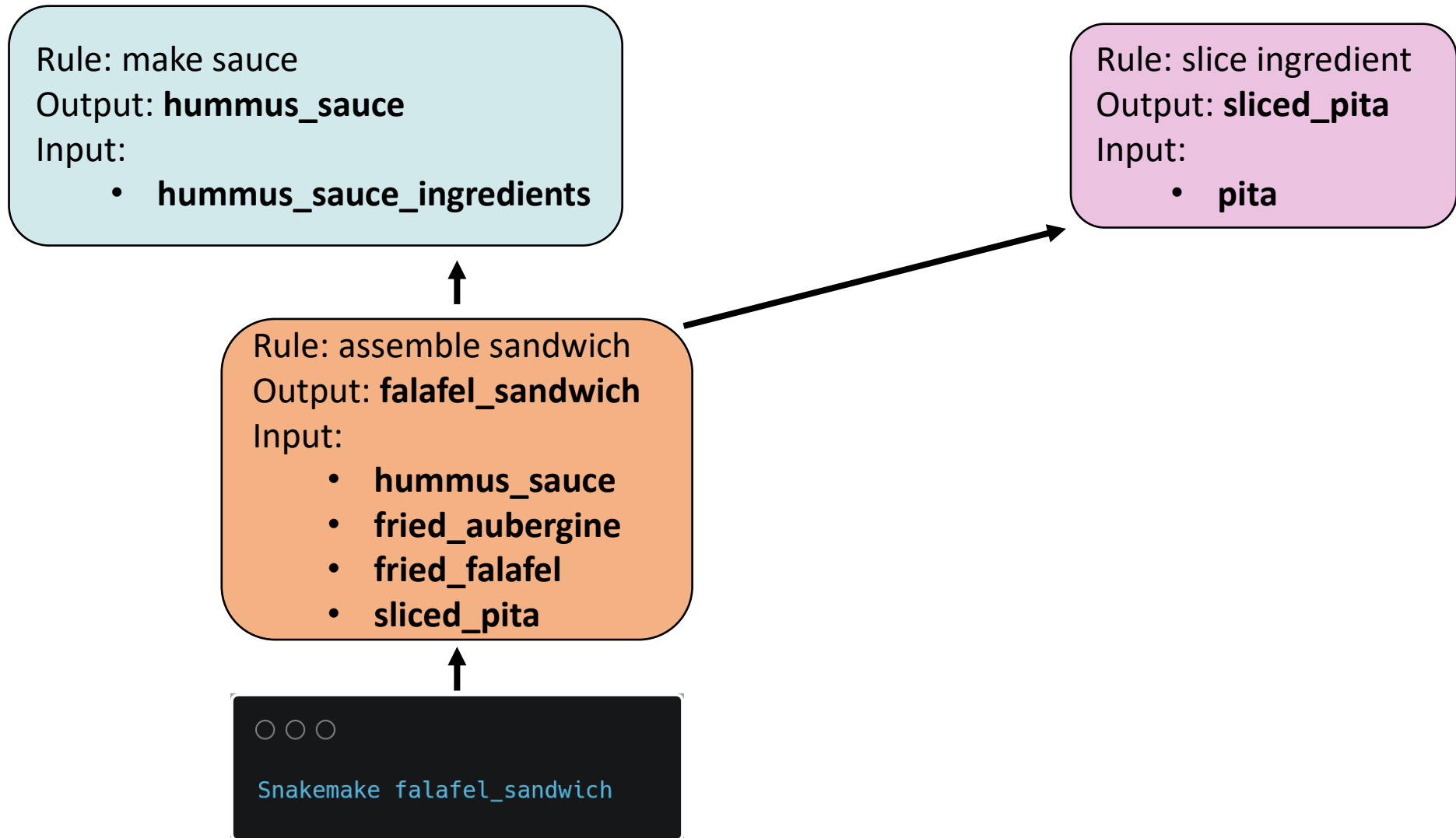
My Middle Eastern friend doesn't like Italian sandwiches...



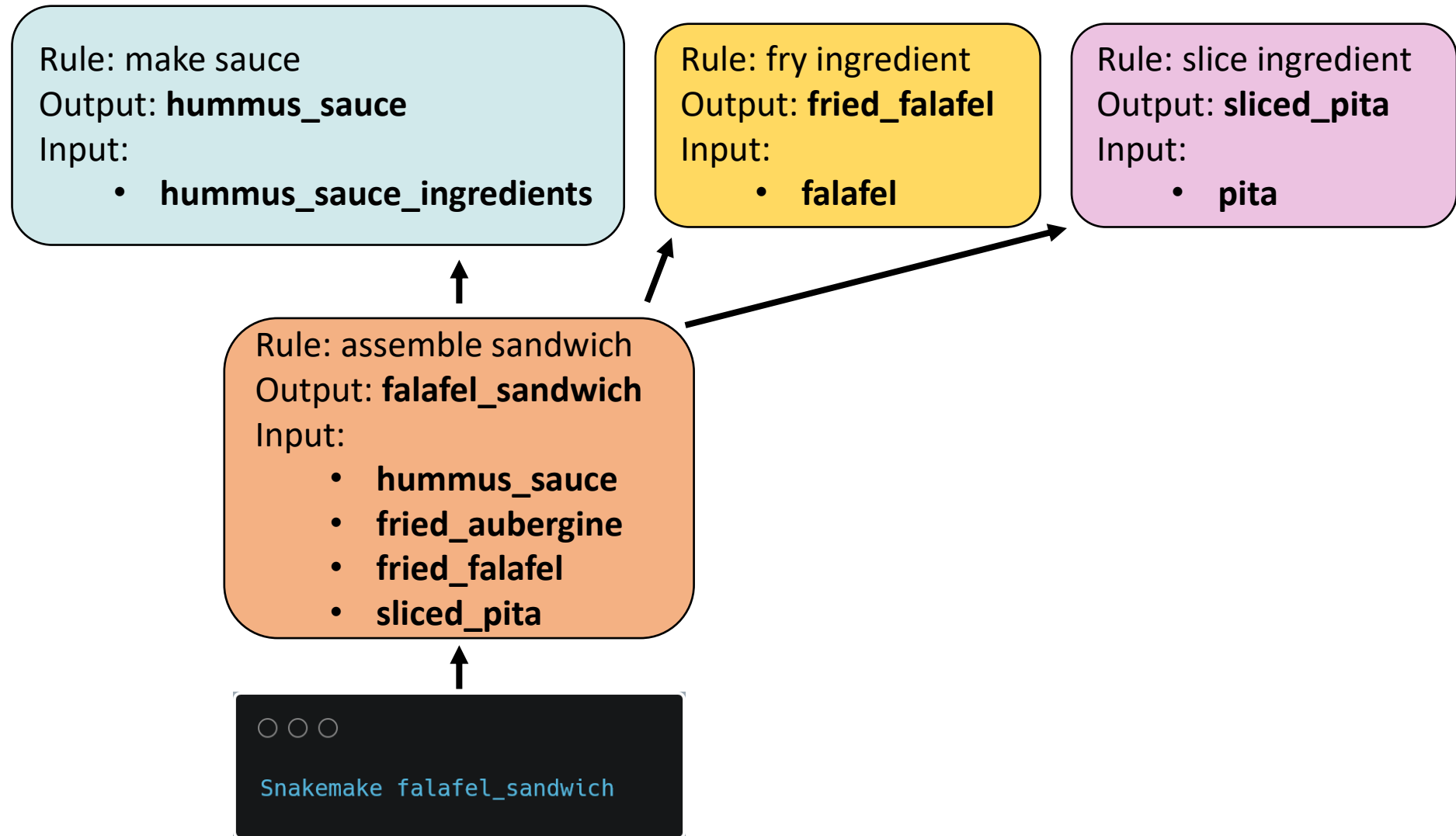
My Middle Eastern friend doesn't like Italian sandwiches...



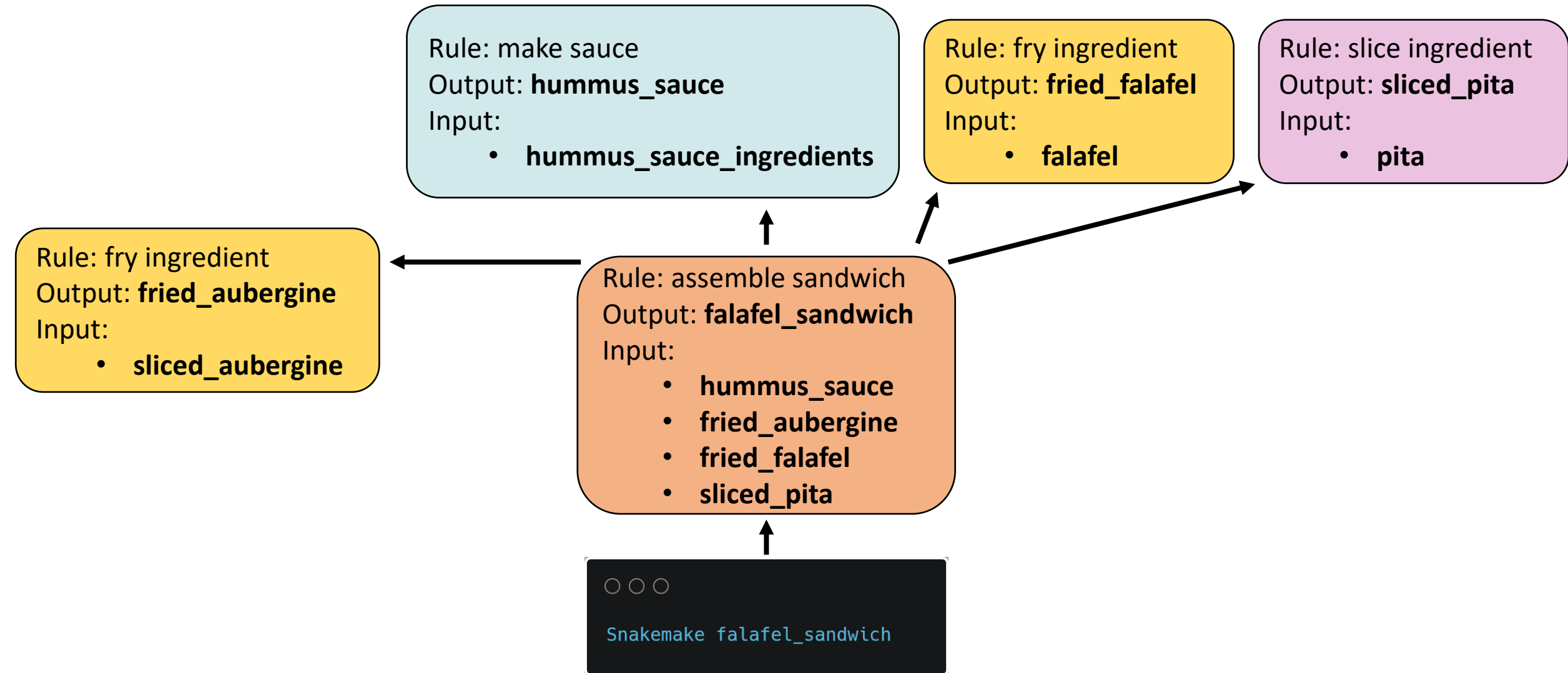
My Middle Eastern friend doesn't like Italian sandwiches...



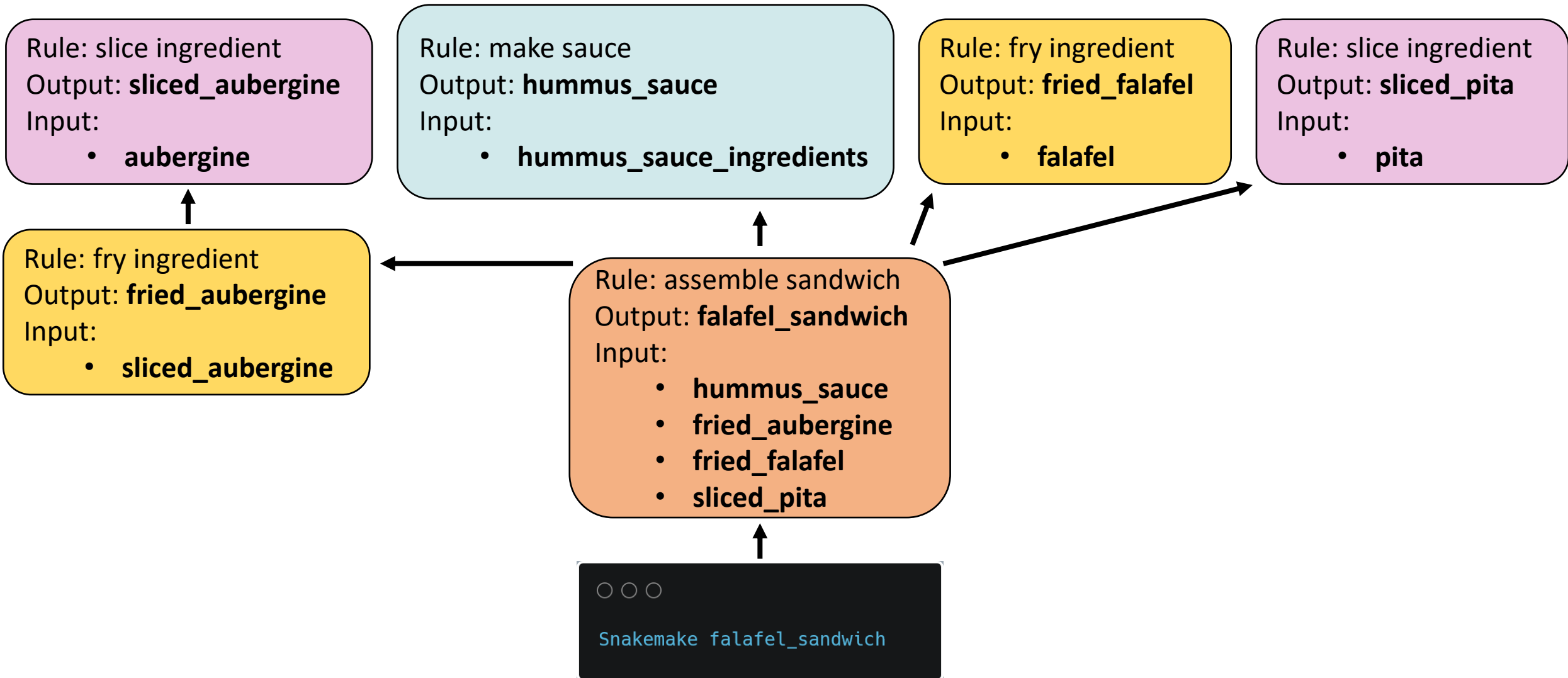
My Middle Eastern friend doesn't like Italian sandwiches...



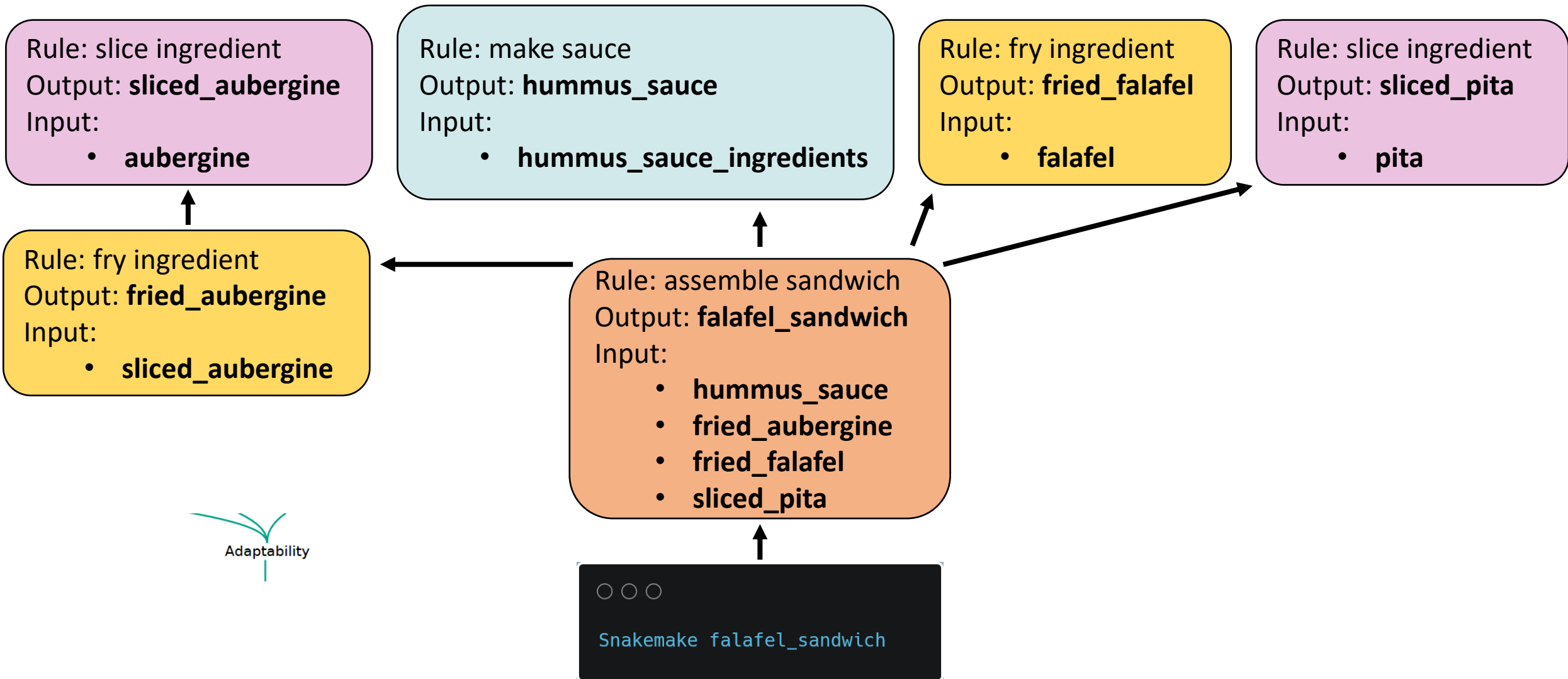
My Middle Eastern friend doesn't like Italian sandwiches...



My Middle Eastern friend doesn't like Italian sandwiches...



My Middle Eastern friend doesn't like Italian sandwiches...



What about the thesis?

What about the thesis?

Rule: assemble thesis

Output: **thesis**

Input:

- **introduction**
- **chapter_1**
- **chapter_2**
- **discussion**

What about the thesis?

Rule: render pdf
Output: **introduction**

Rule: render pdf
Output: **chapter_1**
Input:

- **cool_simulation**

Rule: render pdf
Output: **chapter_2**
Input:

- **awesome_figure**

Rule: render pdf
Output: **discussion**

Rule: assemble thesis
Output: **thesis**
Input:

- **introduction**
- **chapter_1**
- **chapter_2**
- **discussion**

What about the thesis?

Rule: run simulation
Output: **cool_simulation**
Input:

- **cool_theory**

Rule: make figure
Output: **awesome_figure**
Input:

- **awesome_model**

Rule: render pdf
Output: **introduction**

Rule: render pdf
Output: **chapter_1**
Input:

- **cool_simulation**

Rule: render pdf
Output: **chapter_2**
Input:

- **awesome_figure**

Rule: render pdf
Output: **discussion**

Rule: assemble thesis
Output: **thesis**
Input:

- **introduction**
- **chapter_1**
- **chapter_2**
- **discussion**

What about the thesis?

Rule: run simulation
Output: **cool_simulation**
Input:
• **cool_theory**

Rule: make figure
Output: **awesome_figure**
Input:
• **awesome_model**

Rule: render pdf
Output: **introduction**

Rule: render pdf
Output: **chapter_1**
Input:
• **cool_simulation**

Rule: render pdf
Output: **chapter_2**
Input:
• **awesome_figure**

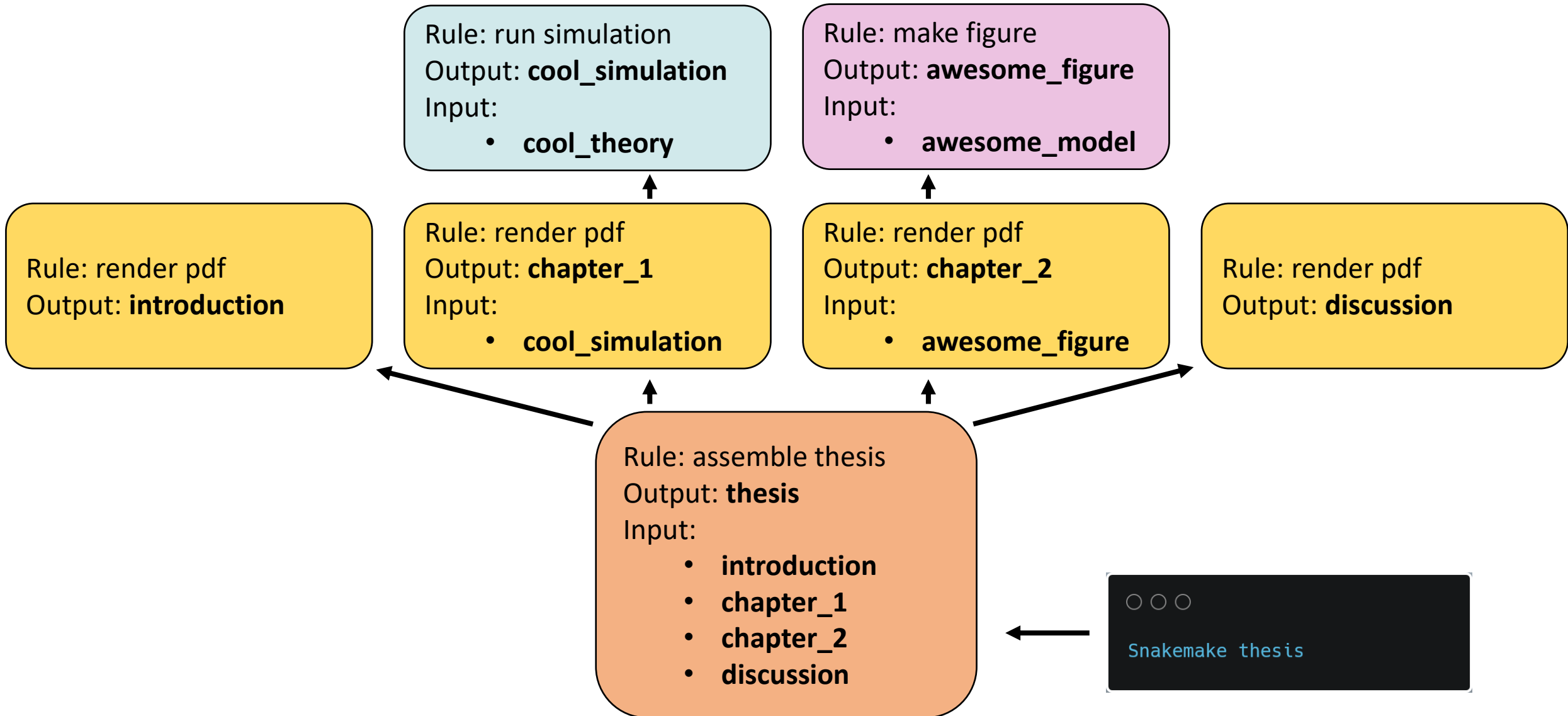
Rule: render pdf
Output: **discussion**

Rule: assemble thesis
Output: **thesis**
Input:
• **introduction**
• **chapter_1**
• **chapter_2**
• **discussion**

○ ○ ○

Snakemake thesis

What about the thesis?



Change is inevitable...

Rule: run simulation
Output: **cool_simulation**
Input:

- **cool_theory**

Rule: make figure
Output: **awesome_figure**
Input:

- **awesome_model**

Rule: render pdf
Output: **introduction**

Rule: render pdf
Output: **chapter_1**
Input:

- **cool_simulation**

Rule: render pdf
Output: **chapter_2**
Input:

- **awesome_figure**

Rule: render pdf
Output: **discussion**

Rule: assemble thesis
Output: **thesis**
Input:

- **introduction**
- **chapter_1**
- **chapter_2**
- **discussion**

Change is inevitable...

Rule: run simulation
Output: **cool_simulation**
Input:

- **cool_theory**

Rule: make figure
Output: **awesome_figure**
Input:

- **awesome_model**

Rule: render pdf
Output: **introduction**

Rule: render pdf
Output: **chapter_1**
Input:

- **cool_simulation**

Rule: render pdf
Output: **chapter_2**
Input:

- **awesome_figure**

Rule: render pdf
Output: **discussion**

Rule: assemble thesis
Output: **thesis**
Input:

- **introduction**
- **chapter_1**
- **chapter_2**
- **discussion**



Change is inevitable...

Rule: run simulation
Output: **cool_simulation**
Input:

- **cool_theory**

Rule: make figure
Output: **awesome_figure**
Input:

- **[awesome_model]**

Rule: render pdf
Output: **introduction**

Rule: render pdf
Output: **chapter_1**
Input:

- **cool_simulation**

Rule: render pdf
Output: **chapter_2**
Input:

- **awesome_figure**

Rule: render pdf
Output: **discussion**

Rule: assemble thesis
Output: **thesis**
Input:

- **introduction**
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Change is inevitable...

Rule: run simulation
Output: **cool_simulation**
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Rule: make figure
Output: **awesome_figure**
Input:

- **[awesome_model]**

Rule: render pdf
Output: **introduction**

Rule: render pdf
Output: **chapter_1**
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Rule: render pdf
Output: **chapter_2**
Input:

- **awesome_figure**

Rule: render pdf
Output: **discussion**

Rule: assemble thesis
Output: **thesis**
Input:

- **introduction**
- **chapter_1**
- **chapter_2**
- **discussion**

○ ○ ○

Snakemake thesis



Change is inevitable...

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Output: **awesome_figure**
Input:
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Input:
• **cool_simulation**

Rule: render pdf
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Input:
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Rule: render pdf
Output: **discussion**

Rule: assemble thesis
Output: **thesis**
Input:
• **introduction**
• **chapter_1**
• **chapter_2**
• **discussion**

○ ○ ○
Snakemake thesis



Rendering the pdf

Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**

Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



○○○

Our figure shows a very significant finding.

```
``` {r}
importing the figure
readRDS('{input.awesome_figure}')
```
```

Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



○ ○ ○

Our figure shows a very significant finding.

```
``` {r}
importing the figure
readRDS('{input.awesome_figure}')
```
```

✓ Updates results automatically

Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



○ ○ ○

Our figure shows a very significant finding.

```
``` {r}
importing the figure
readRDS('{input.awesome_figure}')
```
```

- ✓ Updates results automatically
- ✓ Encourages writing while analysing

Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



○○○

Our figure shows a very significant finding.

```
``` {r}
importing the figure
readRDS('{input.awesome_figure}')
```
```

- ✓ Updates results automatically
- ✓ Encourages writing while analysing
- ✓ Maintains reproducibility, adaptability and transparency

Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



○ ○ ○

Our figure shows a very significant finding.

```
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```
```

- ✓ Updates results automatically
- ✓ Encourages writing while analysing
- ✓ Maintains reproducibility, adaptability and transparency
- ✓ Version-controlled reports

Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



○ ○ ○

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Rendering the pdf

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Output: **chapter_2**

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○○○

Our figure shows a very significant finding.

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```
```

- ✓ Updates results automatically
- ✓ Encourages writing while analysing
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- ✓ Version-controlled reports

✗ Copy-pasting



Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



```
Our figure shows a very significant finding.  
  
`` {r}  
# importing the figure  
readRDS('{input.awesome_figure}')
```

- ✓ Updates results automatically
- ✓ Encourages writing while analysing
- ✓ Maintains reproducibility, adaptability and transparency
- ✓ Version-controlled reports



- ✗ Copy-pasting
- ✗ final_version.docx,
final_version_2.docx

Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



```
Our figure shows a very significant finding.  
  
``` {r}  
importing the figure
readRDS('{input.awesome_figure}')```
```

- ✓ Updates results automatically
- ✓ Encourages writing while analysing
- ✓ Maintains reproducibility, adaptability and transparency
- ✓ Version-controlled reports



- ✗ Copy-pasting
- ✗ final\_version.docx, final\_version\_2.docx
- ✗ “Where is the script that produced this figure?”

# Rendering the pdf

Rule: render pdf

Output: **chapter\_2**

Input:

- **awesome\_figure**



```
○○○

Our figure shows a very significant finding.

``` {r}  
# importing the figure  
readRDS('{input.awesome_figure}')
```

- ✓ Updates results automatically
- ✓ Encourages writing while analysing
- ✓ Maintains reproducibility, adaptability and transparency
- ✓ Version-controlled reports



- ✗ Copy-pasting
- ✗ final_version.docx, final_version_2.docx
- ✗ “Where is the script that produced this figure?”

Templates

Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



```
○○○  
  
Our figure shows a very significant finding.  
  
``` {r}  
importing the figure
readRDS('{input.awesome_figure}')
```

- ✓ Updates results automatically
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- ✓ Version-controlled reports



- ✗ Copy-pasting
- ✗ final\_version.docx, final\_version\_2.docx
- ✗ “Where is the script that produced this figure?”

## Templates



# Rendering the pdf

Rule: render pdf

Output: **chapter\_2**

Input:

- **awesome\_figure**



```
○○○

Our figure shows a very significant finding.

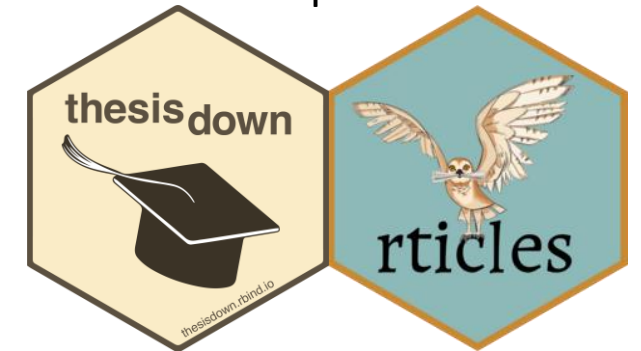
``` {r}  
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- ✗ Copy-pasting
- ✗ final_version.docx, final_version_2.docx
- ✗ “Where is the script that produced this figure?”

Templates



Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



```
○○○  
  
Our figure shows a very significant finding.  
  
{r}  
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readRDS('{input.awesome_figure}')
```

- ✓ Updates results automatically
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- ✗ Copy-pasting
- ✗ final_version.docx, final_version_2.docx
- ✗ “Where is the script that produced this figure?”

Templates



Don't use R?
Hooked on Jupyter notebooks?

Rendering the pdf

Rule: render pdf

Output: **chapter_2**

Input:

- **awesome_figure**



```
○○○  
  
Our figure shows a very significant finding.  
  
{r}  
# importing the figure  
readRDS('{input.awesome_figure}')
```

- ✓ Updates results automatically
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- ✓ Maintains reproducibility, adaptability and transparency
- ✓ Version-controlled reports



- ✗ Copy-pasting
- ✗ final_version.docx, final_version_2.docx
- ✗ “Where is the script that produced this figure?”

Templates



Don't use R?

Hooked on Jupyter notebooks?



Better work with Snakemake & R Markdown

Better work with Snakemake & R Markdown



+



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Better work with Snakemake & R Markdown



+



=

Reproducibility
Adaptability
Transparency

Better work with Snakemake & R Markdown



+



=

Reproducibility
Adaptability
Transparency



Better work with Snakemake & R Markdown



+



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Reproducibility
Adaptability
Transparency



Learn Snakemake:
Carpentries Incubator course



Better work with Snakemake & R Markdown



+



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Reproducibility
Adaptability
Transparency



Learn Snakemake:
Carpentries Incubator course



Learn R Markdown:
R Markdown vignette

