Workflows and ‘wf-*’ Packages

1st ESD Hackathon Heideldberg – 2024-11-26..29

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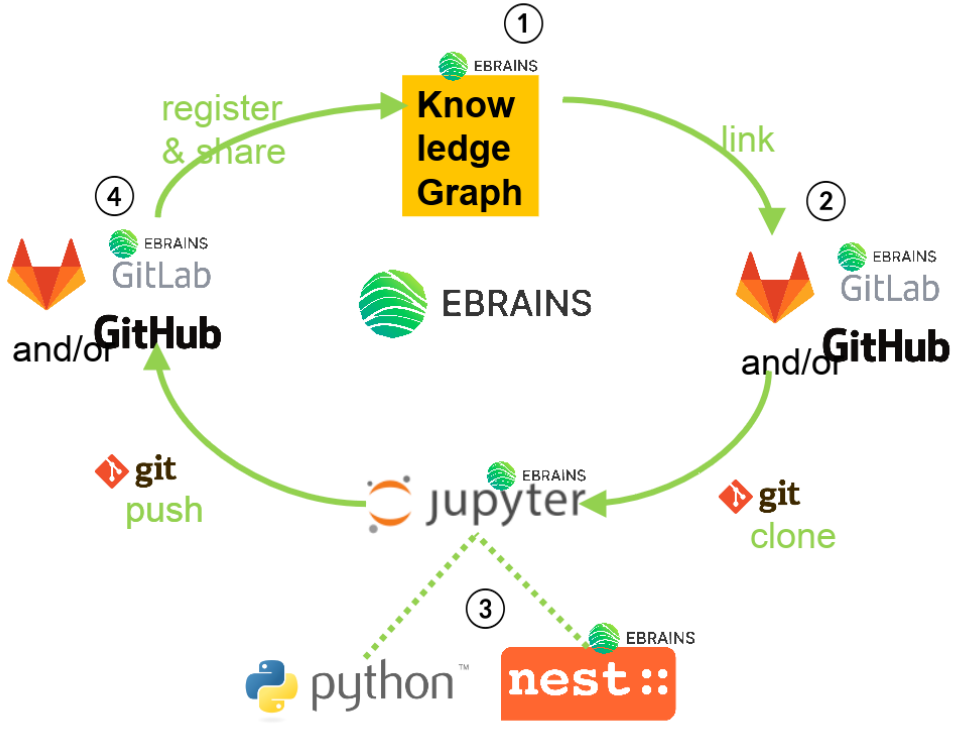
- Model re-use workflow example
- Make it work
    - Single click link
    - dependencies
    - testing (tomorrow)

MODEL RE-USE WORKFLOW EXAMPLE



Alice wants to study dynamical properties of the visual cortex.

1. As the starting point she therefore queries whether a corresponding model is **already available on EBRAINS**.
2. She **transfers it to her own workspace.**
3. After **interactively running and improving** it in Jupyter, she pushes the model back to her repository.
4. Updates **can be merged back** to the original repository and **new releases are published** in the KnowledgeGraph.

(Bernstein Conference 2022, Dennis Terhorst)

Aspects of the example

- central/decentral storage of models and data
    - links and metadata
    - own, group, or public
- installed, reproducible, comparable setup
    - tested, transitive, citable
- exploration and evolution is part of the process
    - access, availability and curation

Applications of the process

- Reproducibility
- Examples for users
- Workshops / tutorials / schools
- Use-cases

Look and feel

Repository README

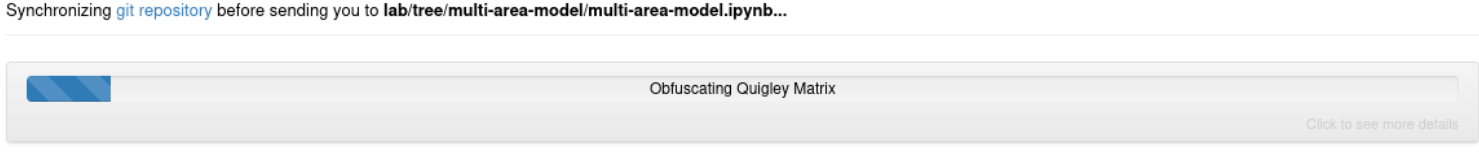
Try it on EBRAINS

Want to start using or simply run the model? Click the button below.
Please note: make sure you check and follow our User instructions, especially if you plan to make and save the changes, or if you simply need step-by-step instructions.

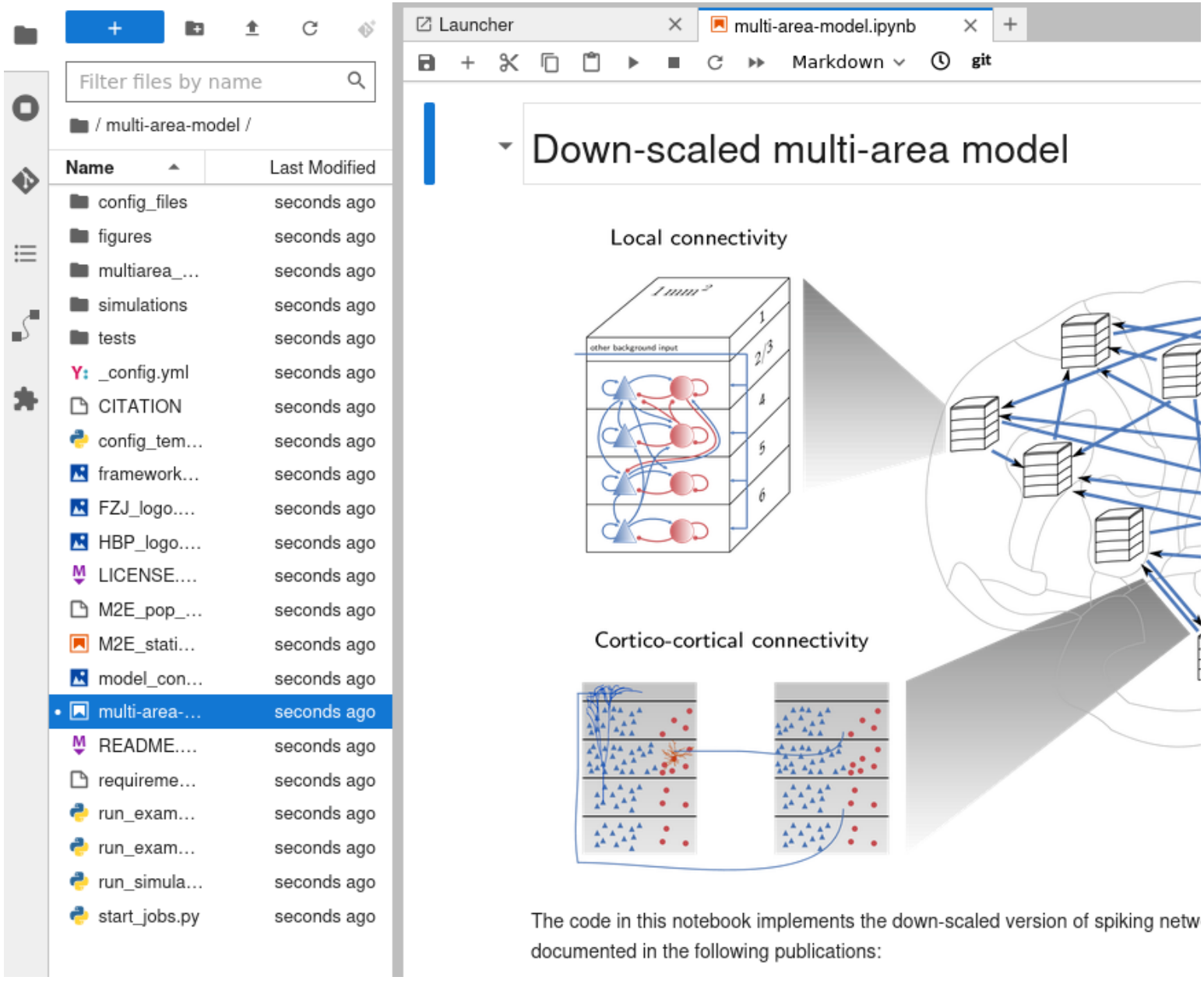
⇒Try it on  EBRAINS

search for the “Multi Area Model”

Jupyter opens



Notebook opens



Additional Notes

How to make it work

Repository

Have a public* repository with your code.

Try it on EBRAINS

Want to start using or simply run the model? Click the button below.
Please note: make sure you check and follow our User instructions, especially if you plan to make and save the changes, or if you simply need step-by-step instructions.

⇒Try it on  EBRAINS

- place a link in your README
- (optionally) use a central image

*) non-public is possible.

Single click link

+ ⇒Try it on EBRAINS

nbgitpuller.readthedocs.io + TryItOnEBRAINS.png

```
[
  ![](https://nest-simulator.org/TryItOnEBRAINS.png)
](https://lab.ebrains.eu/hub/user-redirect/git-pull?repo=https%3A%2F%2Fgithub.com
  %2F...model.ipynb&branch=v1.2
)
```

🎉 works.

nbgitpuller link generator

Use the following form to create your own `nbgitpuller` links.

Note

Consider using the nbgitpuller link generator browser extension instead! Available for Firefox and Chrome.

JupyterHub | Launch from Canvas | Binder

https://lab.ebrains.eu/hub/user-redirect/git-pull?repo=https%3A%2F%2Fgitlab.ebrains.eu%2F Copy

JupyterHub URL: https://lab.ebrains.eu

The JupyterHub to send users to. nbgitpuller must be installed in this hub.

Git Repository URL: https://gitlab.ebrains.eu/my/cool/project

branch: main

Use `main` instead of `master` for new GitHub repositories

File to open: example_1.ipynb

This file or directory from within the repo will open when user clicks the link.

Application to Open:

- ○ Classic Jupyter Notebook
- ○ RetroLab
- ◉ JupyterLab
- ○ RStudio
- ○ Shiny
- ○ Custom URL

Relative URL to redirect user to

Named Server to open: NamedServer

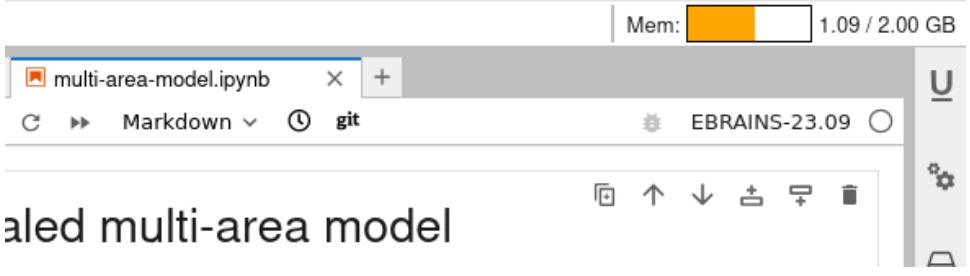
Use for specific named server Jupyter server instance.

Good to know

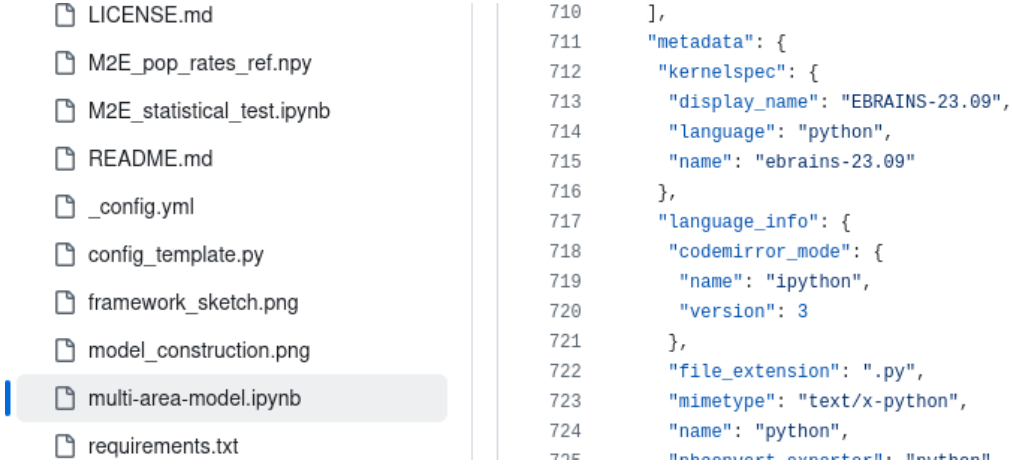
- Point to *releases*, not “main” branch
- Note we didn’t specify the *kernel* to use
- Central image can be changed when EBRAINS decides to change logo or color scheme, etc. (see issue #51 🚧)

Set kernel

Kernel is saved with the notebooks



in the code:



Sanitize dependencies

```
•[1]: !pip install dicthash

[ ]: %matplotlib inline
     import numpy as np
     import sys
     import os
     from IPython.display import display, HTML
```

- no '!pip install …' lines in your notebooks

- know which version *ranges* are likely to work

```
depends_on('py-numpy@:1.16.99', when='@:2.14.99+python', type=
```

Create a ‘wf-*’ package

➡️ https://ebrains.eu/esd → ebrains-spack-builds/packages/wf-*/package.py

```
class WfMultiAreaModel(Package):
    """Meta-package to collect all dependencies of the Multi-Area-Model."""

    homepage="https://inm-6.github.io/multi-area-model/"
    git = "https://github.com/INM-6/multi-area-model"
    maintainer = ["terhorstd", "didi-hou", "rshimoura"]

    version("1.2.0",  tag="v1.2.0")
    version("1.1.1",  tag="v1.1.1")
    version("1.1.0",  tag="v1.1.0")
    version("master",  branch="master")

    depends_on("py-nested-dict", type=("run", "test"))
    depends_on("py-dicthash", type=("run", "test"))
    depends_on("py-matplotlib", type=("run", "test"))
    depends_on("py-numpy", type=("run", "test"))
    depends_on("py-scipy", type=("run", "test"))
    depends_on("py-future", type=("run", "test"))
    depends_on("nest", type=("run", "test"))
    depends_on("py-neo", type=("run", "test"))
    depends_on("py-elephant", type=("run", "test"))
    depends_on("r-aod", type=("run", "test"))
    depends_on("py-notebook", type=("run", "test"))
```

Details

➡️ https://ebrains.eu/esd → ebrains-spack-builds → Wiki

Home

Edit ⋮

Last edited by **Dennis Terhorst** 3 months ago

EBRAINS Software Distribution (ESD)

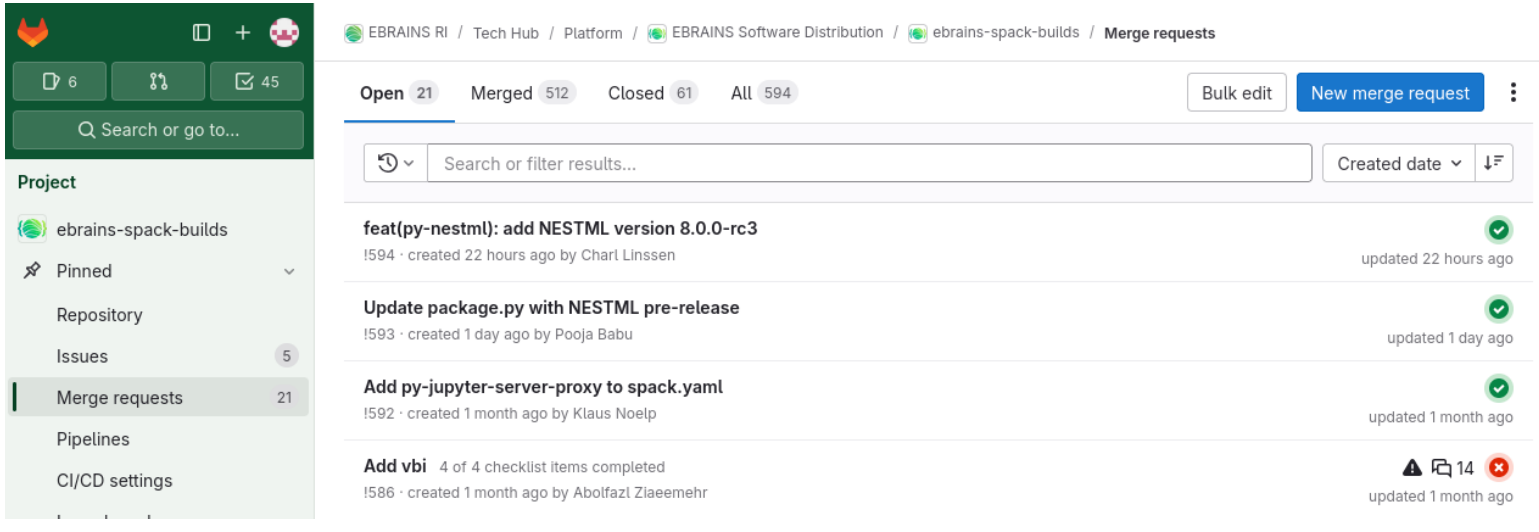
This wiki collects materials around the operational parts of the package definitions, releases and build mechanics.

- Conceptual steering of the work is done in the EBRAINS Software Distribution Integration and Quality work group meetings (aka "ESD meetings").
- HPC deployment related points are discussed in the ESD-on-HPC working group.
- ☑️ Software Quality Checklists

HowTos/Guidelines

- Adding a new EBRAINS tool
- Adding a new EBRAINS wf-package
- Loading the ESD on GitLab CI
- FAQ

Create a merge request



when merged

⏭️ deployment to EBRAINS-experimental kernel next Friday

Summary

- Single line change in your README 🎉
- Understand dependencies
- Declare in a package.py

Next

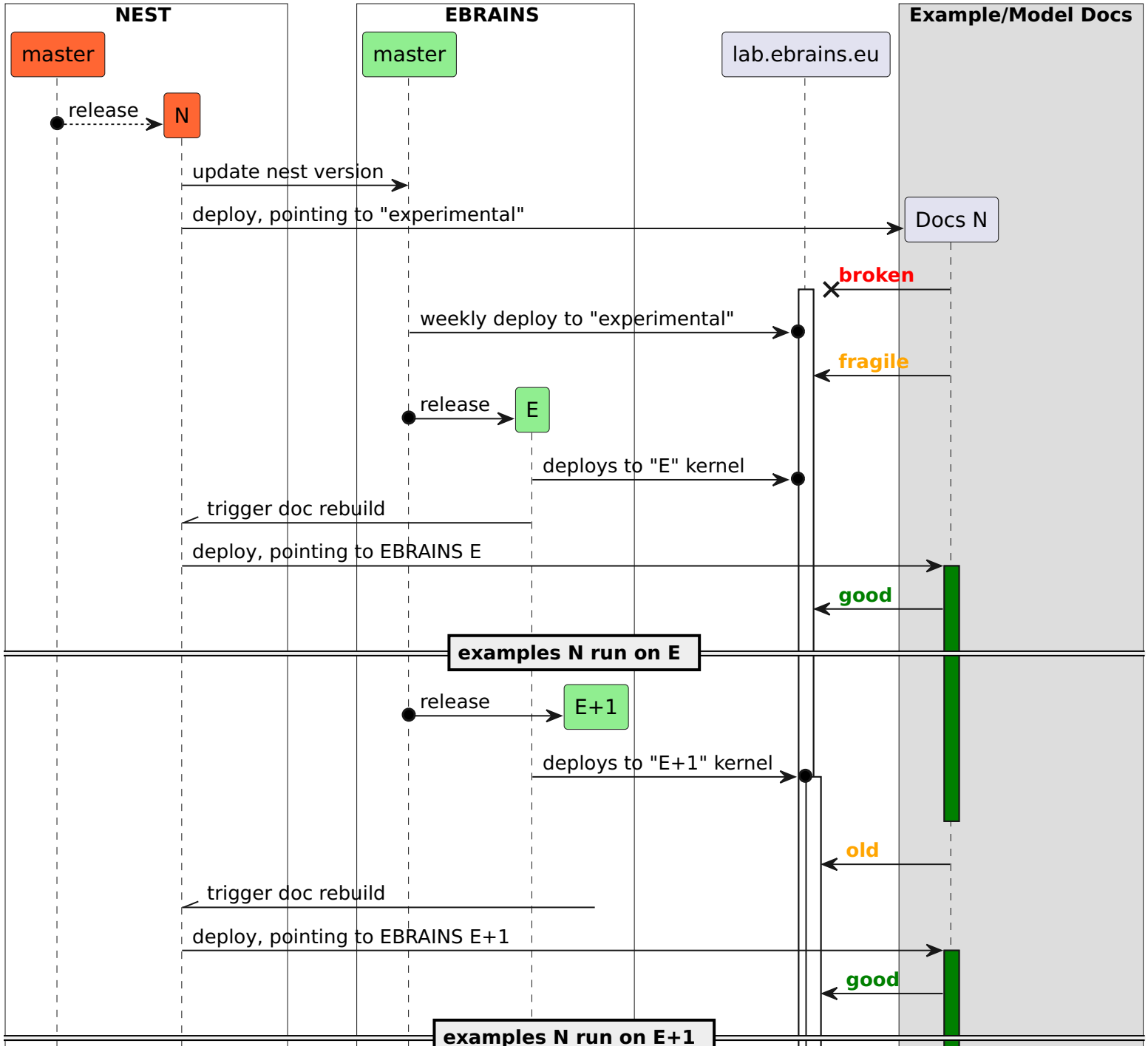
- Version bump and release procedure
- Specify tests (see presentation tomorrow)

Backup

⇒Try it on  EBRAINS **Examples**

- https://nest-simulator.readthedocs.io/en/latest/examples/
- https://github.com/INM-6/multi-area-model
- https://github.com/APE-group/WTA-states

Version bump considerations


NEST
EBRAINS
Example/Model Docs
master
master
lab.ebrains.eu
release
N
update nest version
deploy, pointing to "experimental"
Docs N
broken
weekly deploy to "experimental"
fragile
release
E
deploys to "E" kernel
trigger doc rebuild
deploy, pointing to EBRAINS E
good
examples N run on E
release
E+1
deploys to "E+1" kernel
old
trigger doc rebuild
deploy, pointing to EBRAINS E+1
good
examples N run on E+1