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Continuous Integration with research notebooks: on maintaining reproducibility in atmospheric modeling

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ENVIRONMENTAL
PHYSICS
GROUP

AGH

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OPENATMOS

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Plan of this talk

- Why . . .
  - . . . reproducibility?
  - . . . notebooks?
- open-atmos projects
- Developers' perspective
- Users' perspective
- Summary

What’s next?

- Why . . .
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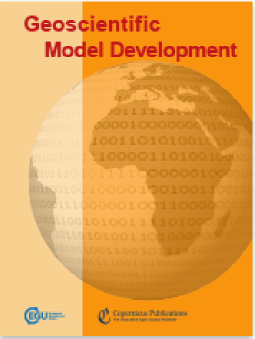
Why reproducibility?



Geoscientific Model Development (GMD) Guidelines[a]

- *“necessary to have access to all of the input data (...)”*

[a] DOI:10.5194/gmd-12-2215-2019

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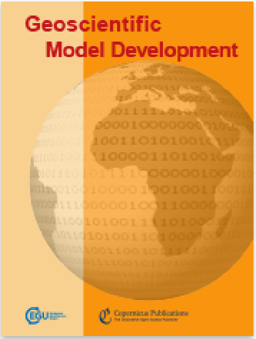

Geoscientific Model Development

Geoscientific Model Development (GMD) Guidelines[a]

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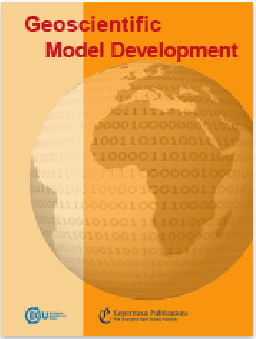

Geoscientific Model Development

Copernicus Publications

Geoscientific Model Development (GMD) Guidelines[a]

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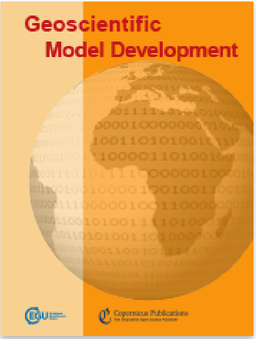

Geoscientific Model Development (GMD) Guidelines[a]

- *“necessary to have access to all of the input data (...)”*
- *“(...) all model configuration files are provided”*
- *“(...) no manual processing of the data”*
- *“All figures and tables must be scientifically reproducible from the scripts”*.

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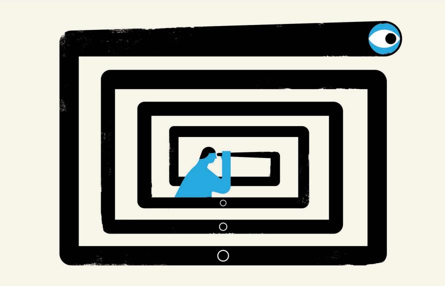
Why notebooks?

“Why Jupyter is data scientists’ computational notebook of choice”

Nature 563 (toolbox): Perkel 2018



- *“We went from Jupyter notebooks not existing some six years ago to in essence everybody using them today”*

Why notebooks?

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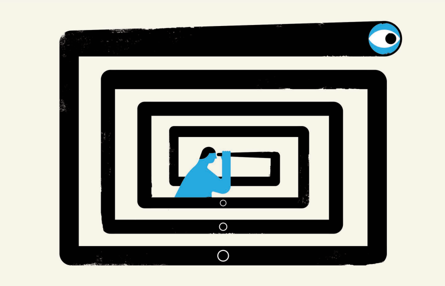
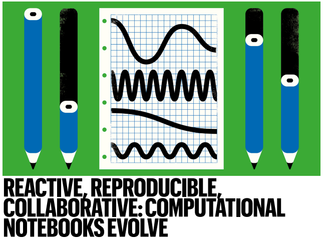


- *“(…) difficult to organize code logically, break it into reusable modules and develop tests to ensure the code is working properly”*

Why notebooks?

Reactive, reproducible, collaborative: computational notebooks evolve

Nature 593: Perkel 2021[2]



REACTIVE, REPRODUCIBLE, COLLABORATIVE: COMPUTATIONAL NOTEBOOKS EVOLVE

- *A 2019 study found that just* **24%** *of 863,878 publicly available Jupyter notebooks on GitHub could be successfully* **re-executed**, *and only* **4%** *produced* **the same results**

[2] (J. F. Pimentel et al. in 2019 IEEE/ACM 16th International Conference on Mining Software Repositories (MSR) 507–517; IEEE, 2019)

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Maintainability

Packages started over 5 years ago serve as good examples for discussion about maintainability.

Projects

PySDM is a **Pythonic high-performance** (multi-threaded CPU & CUDA GPU) implementation of Monte-Carlo **Super-Droplet Method (SDM)** (Shima et al. 2009)

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PySDM

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PyMPDATA

OPENATMOS

open-atmos-jupyter-utils provides utility routines for Jupyter notebooks for: automated testing; presenting visuals; pip-installation of external packages on Colab.

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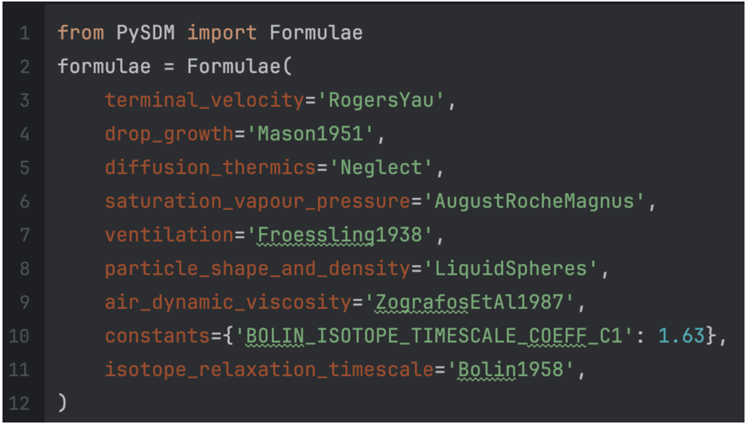
Devs gain

- modularity and IoC
- dimensional analysis
- testing scenarios
- on-boarding new developers

Inversion of Control

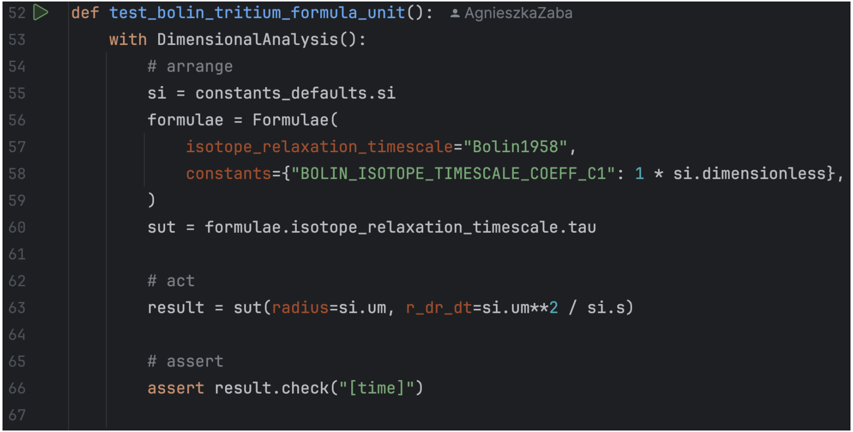
prerequisite for reusability in atmospheric science
and for testing

Atmospheric science: parameterizations and simulation flow control



```
from PySDM import Formulae
formulae = Formulae(
    terminal_velocity='RogersYau',
    drop_growth='Mason1951',
    diffusion_thermics='Neglect',
    saturation_vapour_pressure='AugustRocheMagnus',
    ventilation='Froessling1938',
    particle_shape_and_density='LiquidSpheres',
    air_dynamic_viscosity='ZografosEtAl1987',
    constants={'BOLIN_ISOTOPE_TIMESCALE_COEFF_C1': 1.63},
    isotope_relaxation_timescale='Bolin1958',
)
```

Dimensional analysis of the code



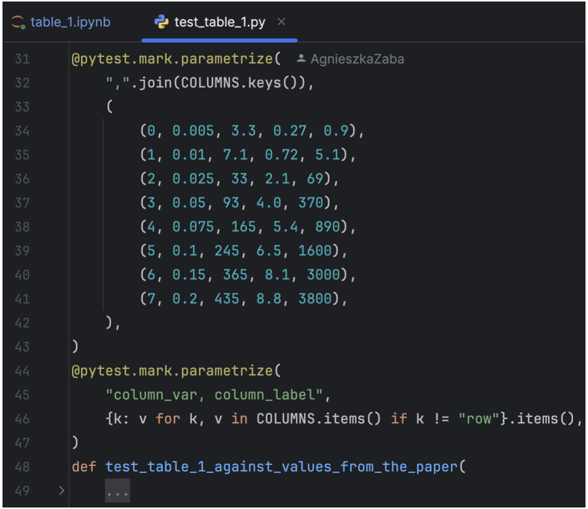
```python
def test_bolin_tritium_formula_unit():  AgnieszkaZaba
    with DimensionalAnalysis():
        # arrange
        si = constants_defaults.si
        formulae = Formulae(
            isotope_relaxation_timescale="Bolin1958",
            constants={"BOLIN_ISOTOPE_TIMESCALE_COEFF_C1": 1 * si.dimensionless},
        )
        sut = formulae.isotope_relaxation_timescale.tau

        # act
        result = sut(radius=si.um, r_dr_dt=si.um**2 / si.s)

        # assert
        assert result.check("[time]")

```

Notebooks as a source of test (edge) cases!

pip install open-atmos-jupyter-utils

notebook_vars()

- executes unmodified notebook code for automated testing
- run-once/multiple asserts (using pytest fixture)



```python
@pytest.mark.parametrize(
    ",".join(COLUMNS.keys()),
    (
        (0, 0.005, 3.3, 0.27, 0.9),
        (1, 0.01, 7.1, 0.72, 5.1),
        (2, 0.025, 33, 2.1, 69),
        (3, 0.05, 93, 4.0, 370),
        (4, 0.075, 165, 5.4, 890),
        (5, 0.1, 245, 6.5, 1600),
        (6, 0.15, 365, 8.1, 3000),
        (7, 0.2, 435, 8.8, 3800),
    ),
)
@pytest.mark.parametrize(
    "column_var, column_label",
    {k: v for k, v in COLUMNS.items() if k != "row"}.items(),
)
def test_table_1_against_values_from_the_paper(
    ...
```

Developers' perspective — DEMO

PySDM

- IoC - formulae chosen by user
- dimensional analysis can be done because of that
- unit tests outside of notebooks
- on-boarding new developers

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Users gain

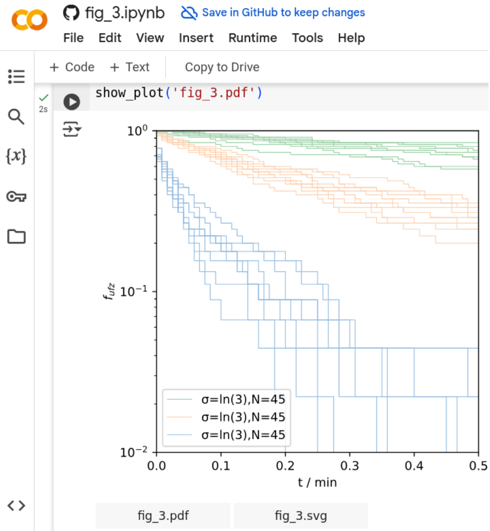
- self-contained notebooks ready to run
- compliance with journal requirements
- maintainable visuals in research-notebooks

Maintainable visuals in research-notebooks

import open_atmos_jupyter_utils

show_plot()

- gives SVG inline graphics
- adds save-SVG/PDF buttons
- Google-Drive link on Colab
- renders OK on GitHub



```
show_plot('fig_3.pdf')
```

Maintainable visuals in research-notebooks

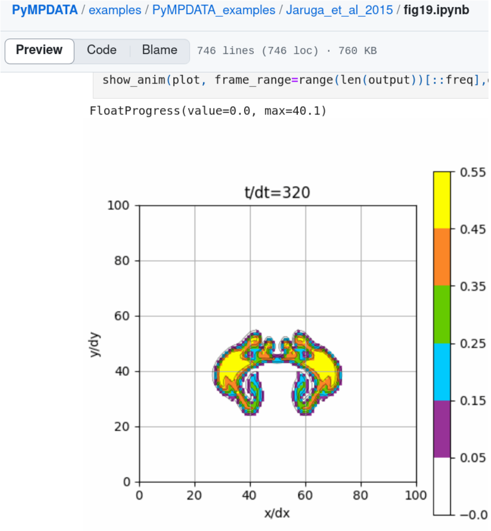
import open_atmos_jupyter_utils

show_plot()

- gives SVG inline graphics
- adds save-SVG/PDF buttons
- Google-Drive link on Colab
- renders OK on GitHub

show_anim()

- uses matplotlib & imageio
- GIF$\rightsquigarrow$base64$\rightsquigarrow$.ipynb JSON
- save-as-GIF button +Colab
- renders OK on GitHub



PyMPDATA / examples / PyMPDATA_examples / Jaruga_et_al_2015 / **fig19.ipynb**

746 lines (746 loc) · 760 KB

```
show_anim(plot, frame_range=range(len(output))[::freq],
```

```
FloatProgress(value=0.0, max=40.1)
```

Users' perspective – DEMO

PyMPDATA

- notebooks are great for tutorials, but only if kept up-to-date with ongoing development (with CI automation!)
- paper-author (compliance with journal requirements) / paper-reviewer perspectives
- maintainable visuals in research-notebooks

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Take home messages

Essential integration

Research notebooks + automated testing workflows

Take home messages

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Modularity and IoC

Benefits for users, developers and on-boarding new contributors

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Generated and embedded visuals

force reproducibility, easier to maintain

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Research notebooks + automated testing workflows

Modularity and IoC

Benefits for users, developers and on-boarding new contributors

Generated and embedded visuals

force reproducibility, easier to maintain

Maintenance of research-result reproducibility

Supports ongoing project development

Acknowledgments

OPENATMOS

NATIONAL SCIENCE CENTRE
POLAND

AGH

RESEARCH UNIVERSITY
EXCELLENCE INITIATIVE

NCAR
MMM

Thank you for your attention!