

Teaching best-practice of open-source collaborative scientific software development

Panel 3: “Educating Future Macro-Energy Systems Researchers”
Macro-Energy Systems Workshop hosted by Stanford Energy

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Background

Starting a new course from scratch...

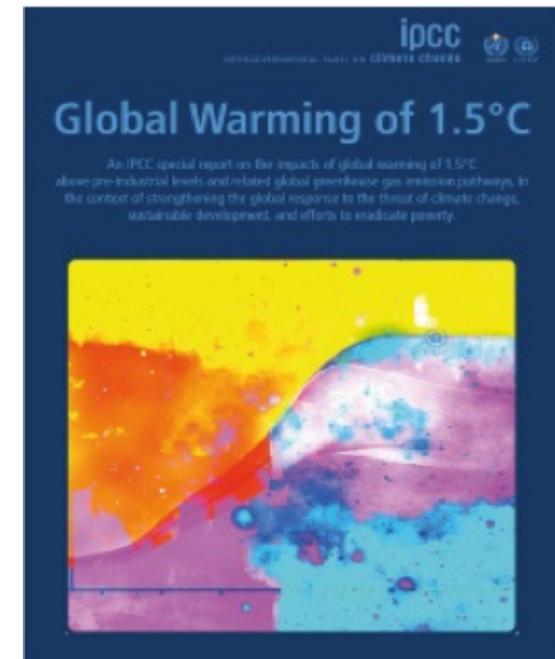
Two years ago, I was asked to create a new course at TU Wien on “open-source energy system modelling” ...

Overview and teaching goals:

- ⇒ Introduction to scientific programming:
open-source software & FAIR data
What is it, why do we it, how do we do it?
- ⇒ Assessment of climate change & sustainable development
How can scenarios be used for analysis in line with open science?
- ⇒ ~~Development of a stylized national energy system model~~
~~How can we develop our own scenarios to analyse policy measures?~~

Not the topic of this talk...

The second part of the lecture is based on my work for the *IPCC Special Report on Global Warming of 1.5°C*
www.ipcc.ch/sr15



Best practice in scientific software development

Concepts that should be familiar to any macro-energy modeller

Overview of concepts discussed in the course (part 1)

- ⇒ Open-source licenses
- ⇒ FAIR principles: Findable, Accessible, Interoperable, Reusable
- ⇒ Git version control & code review (using Github or similar services)
- ⇒ Style guides and documentation
- ⇒ Semantic versioning
- ⇒ Testing and “continuous integration”

Homework assignment (for part 1):

- ⇒ Student uses some code snippet from her/his prior work
- ⇒ Add continuous-integration features (unit testing and style guide validation)

A one-slide guide to open & FAIR research

Even accomplished researchers aren't always up to speed...



DOI:
[10.22022/ene/04-2020.16404](https://doi.org/10.22022/ene/04-2020.16404)

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Five best-practice steps to make your research open & FAIR v1.0
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Five best-practice steps to make your research open & FAIR_{v1.0}



You may think that putting your work* on a website already makes it free & open. But that's not quite true – follow these steps to implement best practice of **#openscience!**

* data sets, text, tables, figures & illustrations, source code, scientific software, ... even #Horizon2020 deliverables

1. Open

If you want your *work to be read, used & shared by others*, be explicit about it: For text, data, figures, ... – use the [CC-BY license](https://creativecommons.org/licenses/by/4.0/) | For code, visit choosealicense.com

2. Findable

To make it easy for others to find and cite your work, get a [digital object identifier \(DOI\)](https://www.doi.org/) and add a *recommended citation*

3. Accessible

Depositing your work in an institutional repository or a service like [zenodo](https://zenodo.org/) ensures that your work is still *available even after the end of the project*

4. Interoperable

Using established community standards, data formats and software packages lets others *quickly understand and use your work*

5. Reusable

To make it easy for others to *build on your work*, make sure to assign a version number and relevant (machine-readable) metadata



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Rationale for open-source research

One can only stand on the shoulders of giants if they let you...

- Science has to be built on transparency and reproducibility
- Describing methods/algorithms with words is a sub-optimal way to share ideas
- Evolution of sharing & openness in the energy modelling community:

🙄 “Available upon reasonable request”

😐 Dumping the final version of a model or scientific software on an institutional server or a service like [GitHub](#) or [Zenodo](#)

😄 Separating the model or scientific software into several modules and making parts open-source as early as possible, writing comprehensive documentation & tutorials, etc.



Rationale for best-practice scientific programming

*Following best-practice principles in your work will give you **more time to do better research***

Modelling and scientific analysis is usually a “constant prototyping” exercise

- ⇒ “Just adding one more feature” often breaks existing functionality
- ⇒ Dependencies (open-source packages) change over time
- ⇒ Models and tools are too complex to immediately notice changed behaviour

Who has not yet experienced the panic & stress from a model not solving shortly before a deadline...?

Following best-practice principles...

- ⇒ Guards against models and tools failing to work (as expected)
- ⇒ Helps you to understand *your own thinking* a few months later

An example of open & FAIR science

The IPCC SR15 as a case study of open & FAIR scenario analysis

Interactive online scenario explorer at data.ene.iiasa.ac.at/iamc-1.5c-explorer

Range of assumptions of socio-economic drivers (Figure 2.4)

Notebook `sr15_2.3.1_range_of_assumptions`

The SR15 SPM and chapters are still undergoing copy-edits and revisions as part of the tricklebacks from the approval plenary. The assessment, statistics tables and figures shown here is therefore still subject to change.

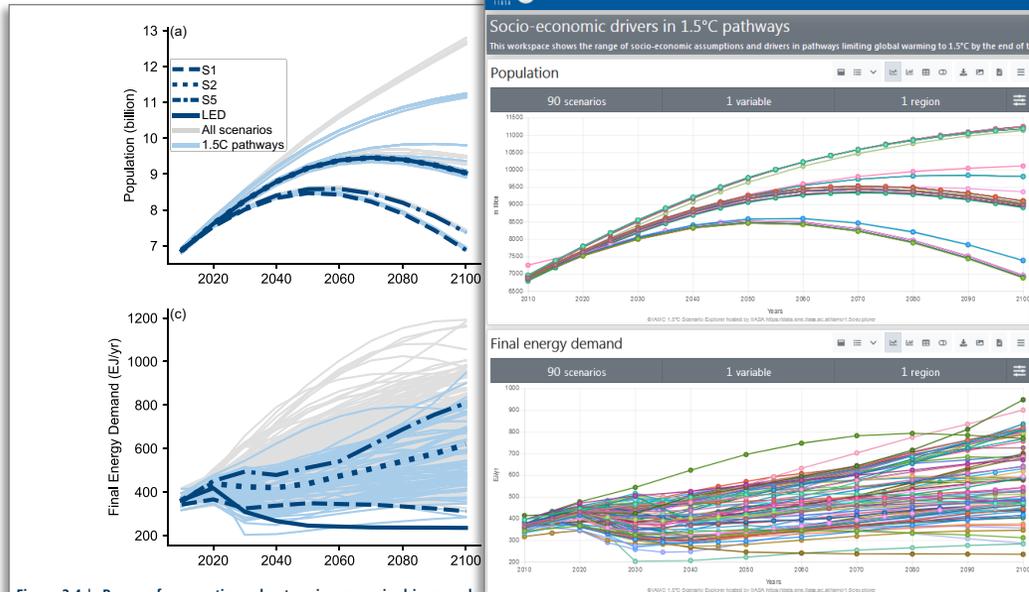


Figure 2.4 | Range of assumptions about socio-economic drivers and assessment. 1.5°C-consistent pathways are blue, other pathways grey. Trajectories for the illustrative 1.5°C-consistent archetypes used in this Chapter (LED, S1, S2, S5; referred to as P1, P2, P3, and P4 in the Summary for Policymakers.) are highlighted. S1 is a sustainability oriented scenario, S2 is a middle-of-the-road scenario, and S5 is a fossil-fuel intensive and high energy demand scenario. LED is a scenario with particularly low energy demand. Population assumptions in S2 and LED are identical. Panels show (a) world population, (b) gross world product in purchasing power parity values, (c) final energy demand, and (d) food demand.

```
In [10]: fig, ax = plt.subplots(2, 2, figsize=(8, 6))

pop = df.filter(variable='Population')
pop.convert_unit({'million': ['billion']})
line_plot_with_markers(ax[0][0], pop,

gdp = df.filter(variable='GDP PPP')
gdp.convert_unit({'billion US$2010/yr': ['billion US$2010/yr']})
line_plot_with_markers(ax[0][1], gdp,

final = df.filter(variable='Final Energy Demand')
line_plot_with_markers(ax[1][0], final,

food = df.filter(variable='Food Demand')
line_plot_with_markers(ax[1][1], food,

ax[0][0].legend(loc=1)
fig.tight_layout()
```

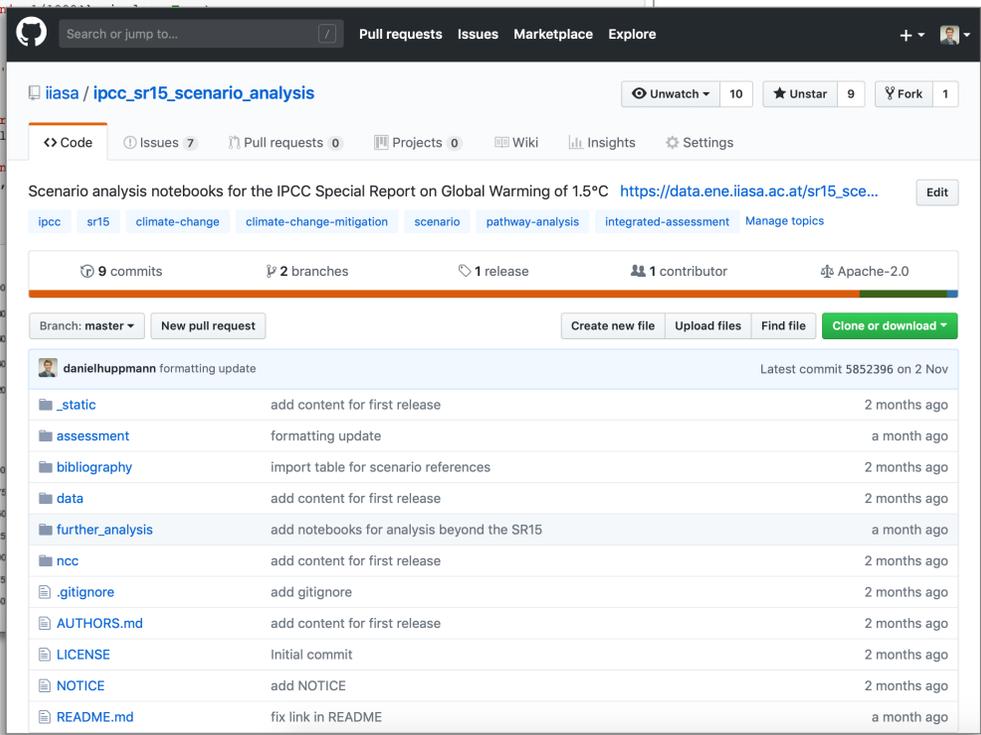
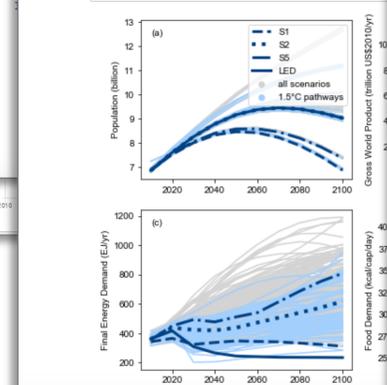


Figure 2.4 as printed in the SR15 (www.ipcc.ch/sr15)

Rendered notebooks to generate figures and tables at data.ene.iiasa.ac.at/sr15_scenario_analysis

```
$ git clone git@github.com:iiasa/ipcc_sr15_scenario_analysis.git
```

The road ahead for macro-energy research

Open science has to go beyond open source...

In an IIASA nexus blog post published today, I discuss how open-source scientific software and FAIR data can bring us one step closer to a community of open science.



⇒ <https://blog.iiasa.ac.at/>

More information on my course at TU Wien (VU 370.062)



⇒ <https://tiss.tuwien.ac.at>

⇒ <https://data.ene.iiasa.ac.at/teaching> (including recording of some lectures)

My plea to the audience of this workshop

⇒ Make teaching resources openly available!



#freethelectures

Thank you very much for your attention!

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Backup slides (for IPCC SR15 analysis)

The IAMC template for timeseries data

A community standard for compiling scenario results



The integrated-assessment community (IAMC) developed a tabular scenario data format for energy systems, SDG dimensions, ...

⇒ Used in IPCC Reports (AR5, SR15), Horizon 2020 projects, EMF, ...

⇒ Adopted by ~50 teams globally

	A	B	C	D	E	F	G	H	
1	Model	Scenario	Region	Variable	Unit	2005	2010	2015	
2	MESSAGE	CD-LINKS 400	World	Primary Energy	EJ/y	462.5	500.7	...	

Current and recent projects:



pyam: a Python package for scenario analysis

An open-source package to facilitate streamlined processing, validation and assessment of scenario results



- Aim: develop a package of useful functions for scenario analysis & visualization following best practice of collaborative scientific software development
- Features:
 - ⇒ Scenario processing workflow (I/O, units, ...)
 - ⇒ Analysis & validation
 - ⇒ Categorization & quantitative indicators
 - ⇒ Visualization features & plotting library
- More information:
 - ⇒ Documentation: pyam-iamc.readthedocs.io
 - ⇒ Scientific reference: M. Gidden and D. Huppmann (2019). Journal of Open Source Software 4(33):1095. doi: [10.21105/joss.01095](https://doi.org/10.21105/joss.01095)

pyam : analysis and visualization of integrated assessment scenarios

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DOI [10.5281/zenodo.1470400](https://doi.org/10.5281/zenodo.1470400) JOSS [10.21105/joss.01095](https://doi.org/10.21105/joss.01095)

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