Build, customize and run models with Xarray-Simlab

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Can we have a single tool that covers all the lifecycle of a scientific idea, from data collection to publication?

Matthias Bussonnier, Jupyter talk @ UC Berkeley, September 2015

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model run

numerical experiment

Matthias Bussonnier, Jupyter talk @ UC Berkeley, September 2015

Xarray-Simlab

- Python framework for *interactive, exploratory and scalable* modelling
- Tightly integrated with 

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& friends
- Domain-agnostic
  - Geomorphology, hydrology, ecosystem modelling...

- Project started in 2017, (im)mature

https://github.com/xarray-contrib/xarray-simlab

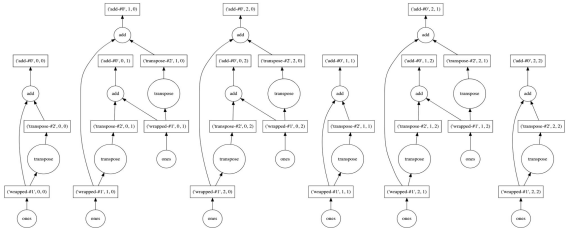
Inspired by

Domain-specific modelling frameworks (Python)

CLIMLAB

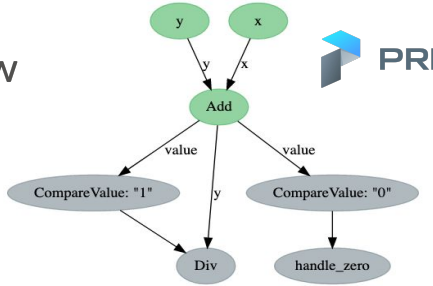
Workflow / task management libraries and frameworks (DAGs everywhere)

DASK



Apache Airflow

luigi

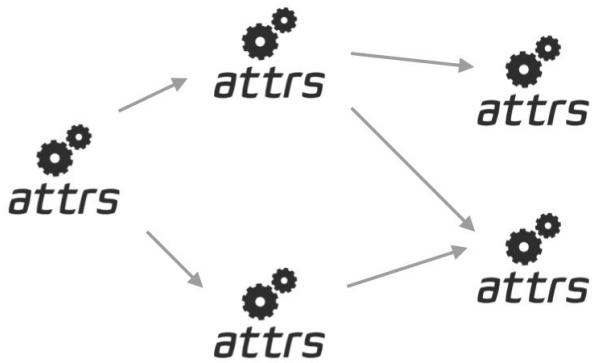


PREFECT

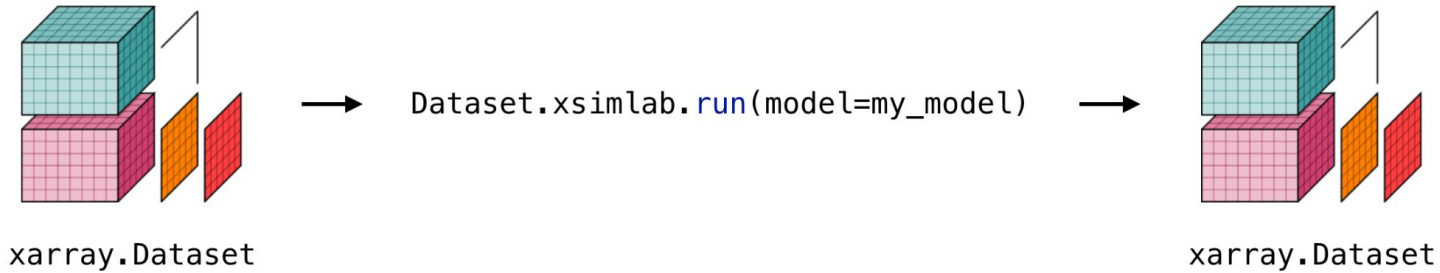
A Model = a collection of “dataclasses” called processes

With implicit DAG (re)construction

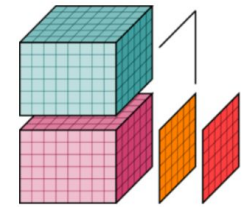
```
my_model = xsimlab.Model({                                    })
```



Simulation(s): Dataset IN, Dataset OUT

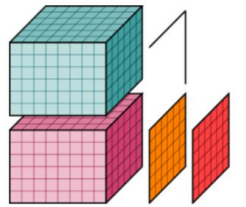


Simulation(s): Dataset IN, Dataset OUT



xarray.Dataset

```
(Dataset
 .<some_preprocessing>
 .xsimlab.run(model=my_model)
 .<some_postprocessing>)
```



xarray.Dataset

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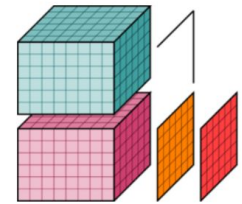
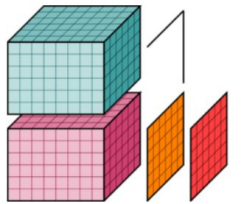


xarray.Dataset

```
Dataset.xsimlab.run(
    model=my_model,
    batch_dim="batch",
    parallel=True,
    store="run.zarr"
)
```



xarray.Dataset

DASK

Zarr

DEMO

Many more features

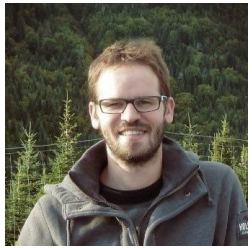
- Model customization by process class inheritance
- Execute the DAG of process classes in parallel with Dask
- Flexible variable dimensions
- Other kinds of variables (group, on_demand, etc.)
- Time-varying input values
- Simulation monitoring and control via hooks
- Zarr encoding options

What's next?

- Explicit process dependencies (ongoing, @Joeperdefloep)
    - Will enable workflows more familiar to modellers...
- More flexible simulation stages
    - Xarray-centric data workflow system? (one "run" stage)
- Command-line and/or graphical (Jupyter widgets) interface
- More users and contributors from various domains! (hopefully)

Thank you for your attention!

Xarray-simlab: https://github.com/xarray-contrib/xarray-simlab



@benbovy