`nbscuid`: Towards a CESM Diagnostics Workflow Built on Jupyter Notebooks

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Introducing the workflow

Goals

- Notebook-based for easy sharing and annotating, with support for scripts for back-compatibility
- Flexible diagnostic framework - run out of the box or customize
- Catalog-friendly for simpler data access
- Multiple options for computational resources

Intro

README.md

nbscuid

Notebook-Based, Super CUstomizable Infrastructure for Diagnostics

Installation

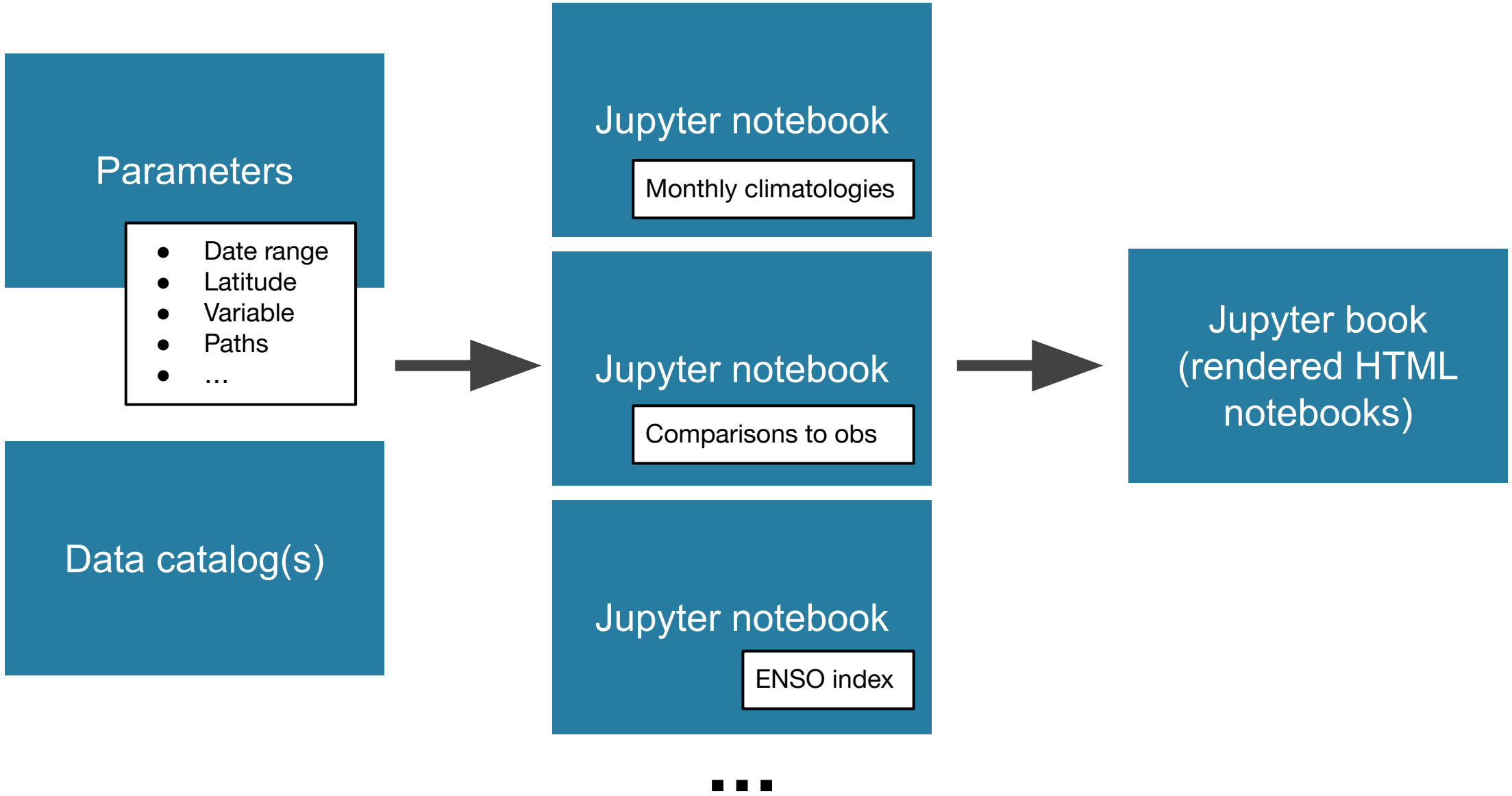
- Run:

```
pip install nbscuid
```

This is a package to enable running notebook-based diagnostic workflows. Based on my-cesm-experiment by matt-long: https://github.com/matt-long/my-cesm-experiment.

See some examples of workflows at https://github.com/rmshkv/nbscuid-examples. For a basic tutorial, follow https://nbscuid.readthedocs.io/en/latest/tutorialsetup.html.

Workflow overview



Tool stack

- **papermill** for parameterizing and executing notebooks
- **jinja** for parameterizing Markdown cells
- **dask** for parallelization
- **intake-esm** for catalog parsing
- **esm_catalog_utils** (cc Keith Lindsay) for catalog creation
- **jupyter book** for turning Jupyter notebooks into publishable HTML

Executing a diagnostic collection

config.yml

- data catalog
- path to template notebooks
- global params
- notebook-specific params
- Jupyter Book config

```
nbscuid-run
config.yml
```

- passes params to notebooks
- executes notebooks through **papermill**

Set of executed notebooks

```
nbscuid-build
config.yml
```

Jupyter book

Demo

https://github.com/rmshkv/nbscuid-examples

Demo - backup

```
(base) crhtc47:~/codes/nbsc...smworkshop-demo> nbscuid-run config.yml
/glade/work/eromashkova/miniconda3/lib/python3.9/site-packages/distributed/node.py:183: UserWarning: Port 8787 is already in use.
Perhaps you already have a cluster running?
Hosting the HTTP server on port 41350 instead
  warnings.warn(
Waiting for Dask workers....

Executing /glade/u/home/eromashkova/codes/nbscuid-examples/cesmworkshop-demo/nblibrary/index.ipynb
Executing: 100%|                                                                                | 4/4 [00:02<00:00,  1.84cell/s]
Executing /glade/u/home/eromashkova/codes/nbscuid-examples/cesmworkshop-demo/nblibrary/global_TS_levels.ipynb
Executing:  43%|                                                                                | 10/23 [00:07<00:06,  2.02cell/s]
```

```
(base) crhtc47:~/codes/nbsc...smworkshop-demo> nbscuid-build config.yml

================================================================================

Your _build directory has been emptied except for .jupyter_cache

================================================================================

Running Jupyter-Book v0.15.1
Source Folder: /glade/u/home/eromashkova/codes/nbscuid-examples/cesmworkshop-demo/computed_notebooks/cesmworkshop-demo-run1
Config Path: /glade/u/home/eromashkova/codes/nbscuid-examples/cesmworkshop-demo/computed_notebooks/cesmworkshop-demo-run1/_config.yml
Output Path: /glade/u/home/eromashkova/codes/nbscuid-examples/cesmworkshop-demo/computed_notebooks/cesmworkshop-demo-run1/_build/html
Running Sphinx v4.5.0
making output directory... done
```

Demo - backup

Example project

Diagnostic notebooks

Temperature and salinity biases at selected depth levels

```
import warnings
warnings.filterwarnings("ignore")
```

```
Basemap module not found. Some regional plots may not function properly
```

```
# Empty cell with "parameters" tag, papermill-provided parameters will be inserted below.
```

```
# Parameters
diag_config_yml = {
    "Avg": {"end_date": "0061-12-31", "start_date": "0031-01-01"},
    "Case": {
        "CASEROOT": "/glade/work/gmarques/cesm.cases/G/gmom.e23.GJRAv4.TL319_t061_zstar_N65.nuopc.HBD.
        "CIMEROOT": "/glade/work/gmarques/cesm.sandboxes/cesm2_3_alpha08a.sbx/cime/",
        "OCN_DIAG_ROOT": "/glade/work/gmarques/Notebooks/for_elena/ncfiles/",
        "SNAME": "HBD_zstar",
    },
}
sname = "cesmworkshop-demo-run1"
test_param = "This parameter was inserted!"
woa_path = "/glade/u/home/gmarques/Notebooks/CESM_MOM6/WOA18_remapping/"
WOA18_temp_path = "/glade/u/home/gmarques/Notebooks/CESM_MOM6/WOA18_remapping/WOA18_TEMP_tx0.66v1_34le
WOA18_salt_path = "/glade/u/home/gmarques/Notebooks/CESM_MOM6/WOA18_remapping/WOA18_SALT_tx0.66v1_34le
cluster_scheduler_address = None
subset_kwargs = {}
```

Demo - backup

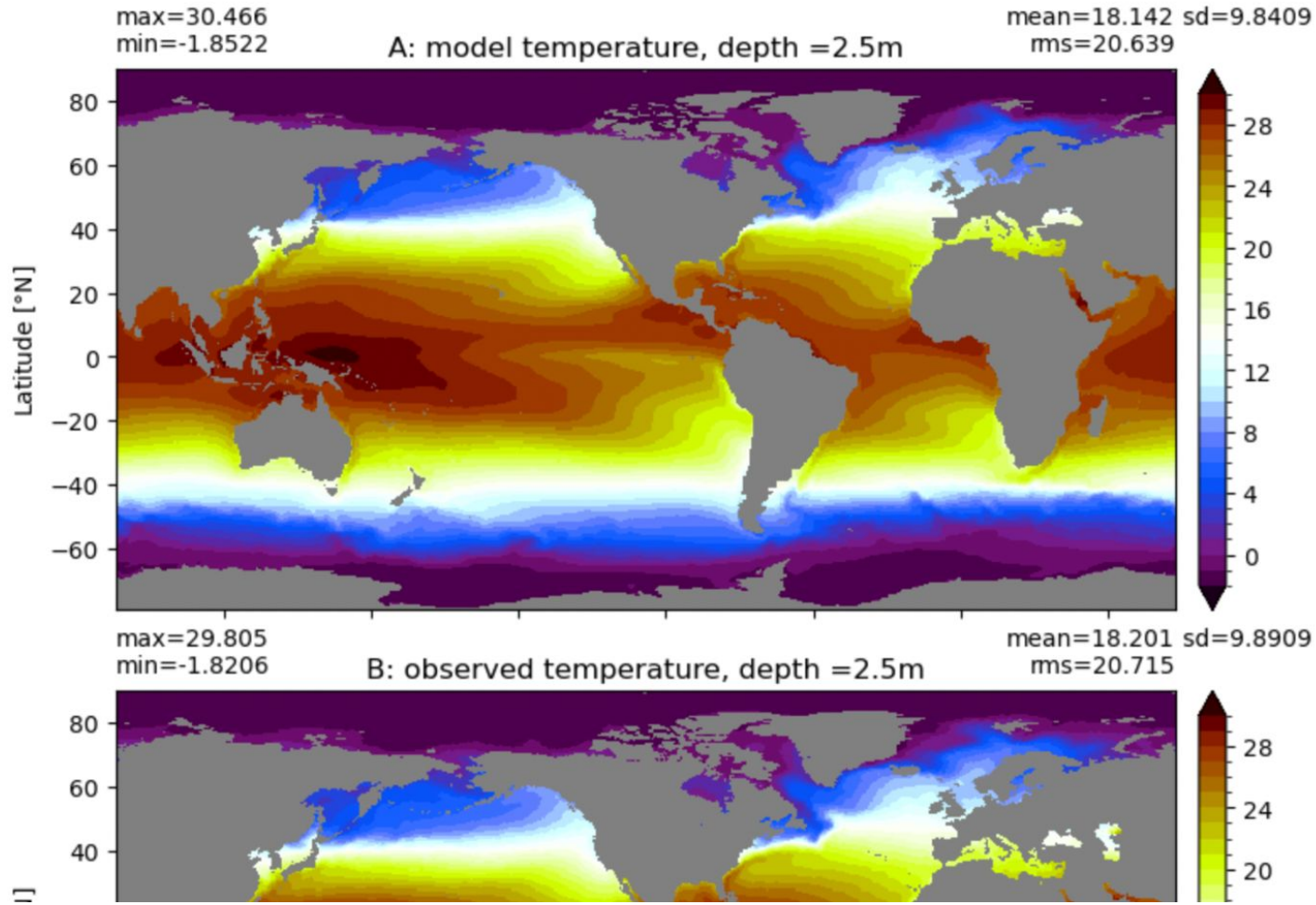
Example project

Diagnostic notebooks

Temperature and salinity biases at selected depth levels

```
            suptitle=dcase.casename + ', averaged '+str(start_date)+ ' and ' +str(end_date),
            clim=(-1.9,30.), dcolormap=plt.cm.bwr,
            extend='both', dextend='neither', dlim=(-2,2),
            show= True)
```

gmom.e23.GJRAv4.TL319_t061_zstar_N65.nuopc.HBD.002, averaged 0031-01-01 and 0061-12-31



Other features

- Run out of the box with a premade config.yml, or customize your own
- Can run any kind of notebook, not just CESM diagnostics
- Run a single notebook on different sets of parameters
- Run notebooks in different environments
- Cache results

Current work and open questions

Experimenting with MOM6 diagnostics

- Current workflow:
  - Diagnostic functions: **mom6-tools**
  - Series of python scripts configured by a yaml file and submitted via bash script through **qsub**
  - Create output files that are displayed through notebooks in **mom6_solutions**
- Goal: converting these diagnostics to be compatible

Next steps to implement

- Executing diagnostics in parallel
- Running non-notebook diagnostics (like .py files)

Managing computational resources

Currently:

- Create a “global” dask cluster on Casper
  - Wait for at least one worker to appear
  - Pass its scheduler address to each notebook
- Each notebook creates a client and attaches it to the global cluster
- Notebooks run in serial

Want:

- Notebooks run in parallel
- Running locally and on non-NCAR machines

Leveraging existing data pipeline packages?

- **Ploomber** - parallelizing notebooks, capability to run Python scripts, creating a more complex task graph to pass data more flexibly between diagnostics elements
- Potentially others - suggestions welcome!

Joining efforts with other CESM diagnostics?

- Currently several diagnostics efforts around NCAR
- Potential collaboration with ADF

Links

Main repo:
https://github.com/rmshkv/nbscuid

Docs: https://nbscuid.readthedocs.io

Usage examples:
https://github.com/rmshkv/nbscuid-examples

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