Enhancing Scientific Reproducibility and Software Correctness in CrocoDash for Regional Ocean Modeling

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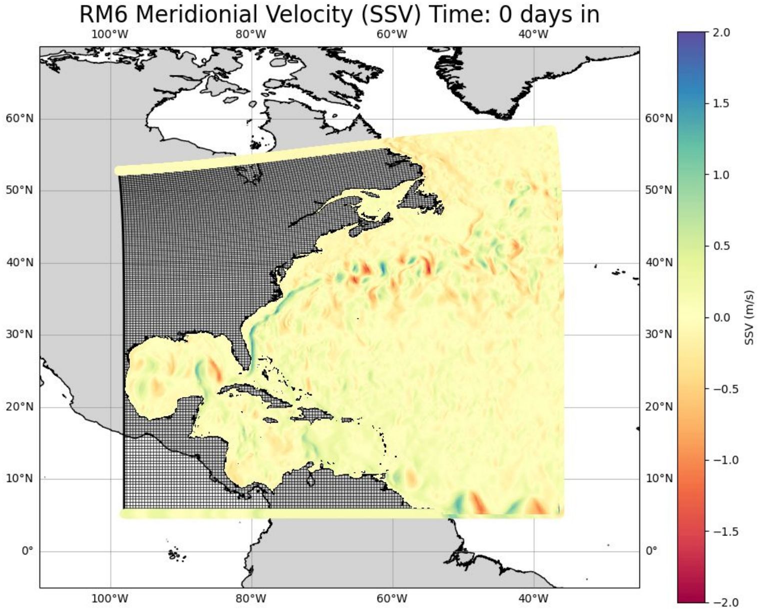
BACKGROUND

Regional ocean models are **powerful** tools.

It can be time-consuming to set these models up.

CESM Regional Ocean and Carbon cOnfigurator with Data assimiLation and Embedding
CROCODILE



Months/Weeks → Days/Hours

PROJECT OBJECTIVE

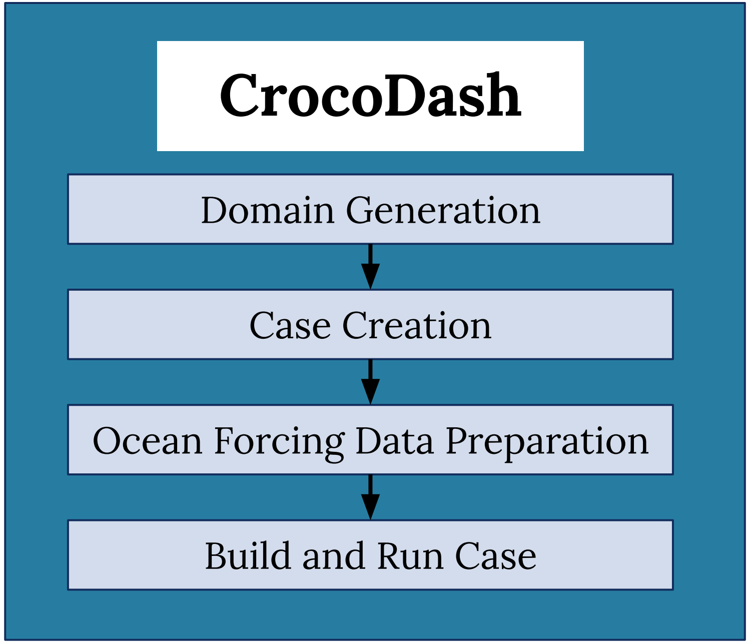
Enhance **scientific reproducibility** and increase **accessibility** in the CrocoDash workflow.

Goal: Fully reproducible end-to-end workflow to create regional Modular Ocean Model version 6 (MOM6) cases!

Case: A specific instance of a model simulation in the Community Earth System Model (CESM).

Domain: Specific region being simulated, including a horizontal grid, vertical grid, and topography.

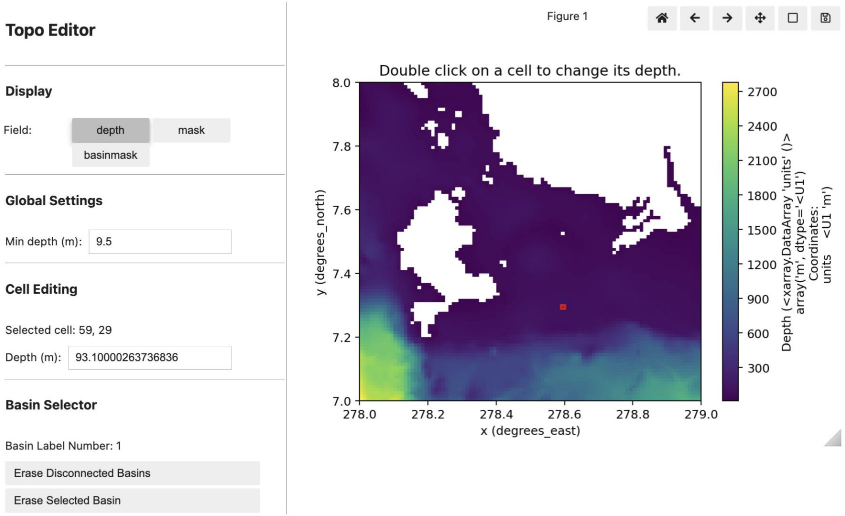
Forcings: Initial conditions (ICs), open boundary conditions (OBCs), tides, and chlorophyll.



MOTIVATION

Model setups are now more user-friendly and streamlined in this workflow but…

There is a lack of **reproducible** features in CrocoDash!



Topo Editor

Display

Field: depth | mask | basinmask

Global Settings

Min depth (m): 9.5

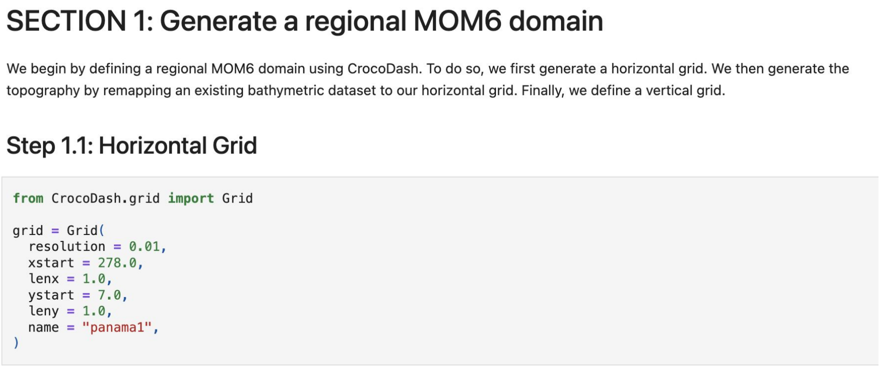
Cell Editing

Selected cell: 59, 29

Depth (m): 93.10000263736836

Basin Selector

Basin Label Number: 1



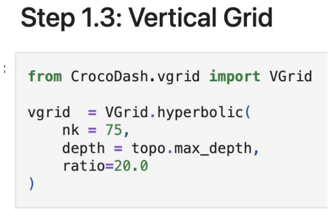
SECTION 1: Generate a regional MOM6 domain

We begin by defining a regional MOM6 domain using CrocoDash. To do so, we first generate a horizontal grid. We then generate the topography by remapping an existing bathymetric dataset to our horizontal grid. Finally, we define a vertical grid.

Step 1.1: Horizontal Grid

```
from CrocoDash.grid import Grid

grid = Grid(
  resolution = 0.01,
  xstart = 278.0,
  lenx = 1.0,
  ystart = 7.0,
  leny = 1.0,
  name = "panama1",
)
```



Step 1.3: Vertical Grid

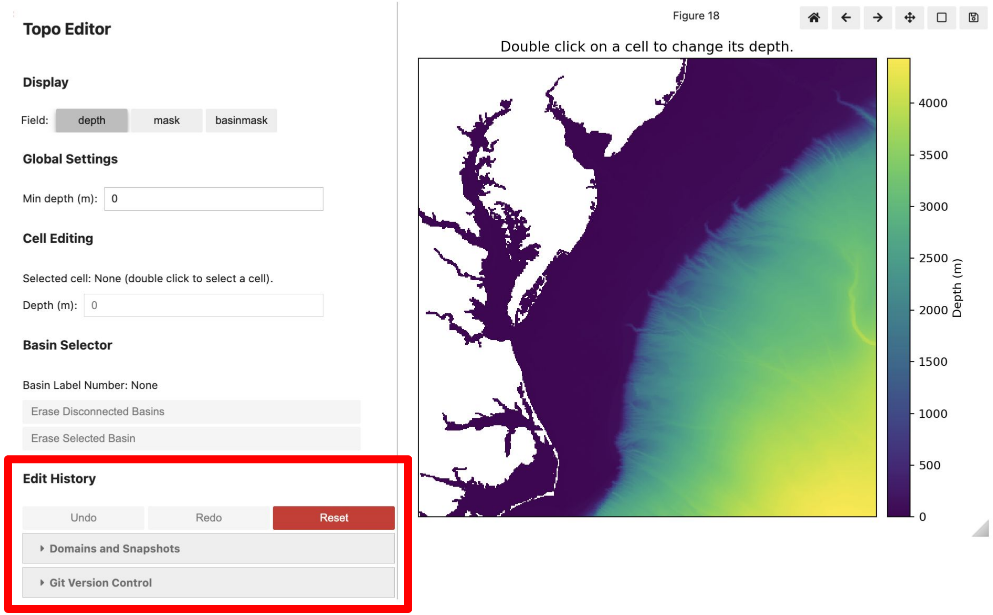
```
from CrocoDash.vgrid import VGrid

vgrid  = VGrid.hyperbolic(
    nk = 75,
    depth = topo.max_depth,
    ratio=20.0
)
```

How do we make this workflow **reproducible**?

SCIENTIFIC REPRODUCIBILITY

Reproducibility = Repeatability + Traceability + Transparency



Topo Editor

Display

Field: depth | mask | basinmask

Global Settings

Min depth (m): 0

Cell Editing

Selected cell: None (double click to select a cell).

Depth (m): 0

Basin Selector

Basin Label Number: None

Erase Disconnected Basins

Erase Selected Basin

Edit History

Undo | Redo | Reset

▸ Domains and Snapshots

▸ Git Version Control

Figure 18

Double click on a cell to change its depth.

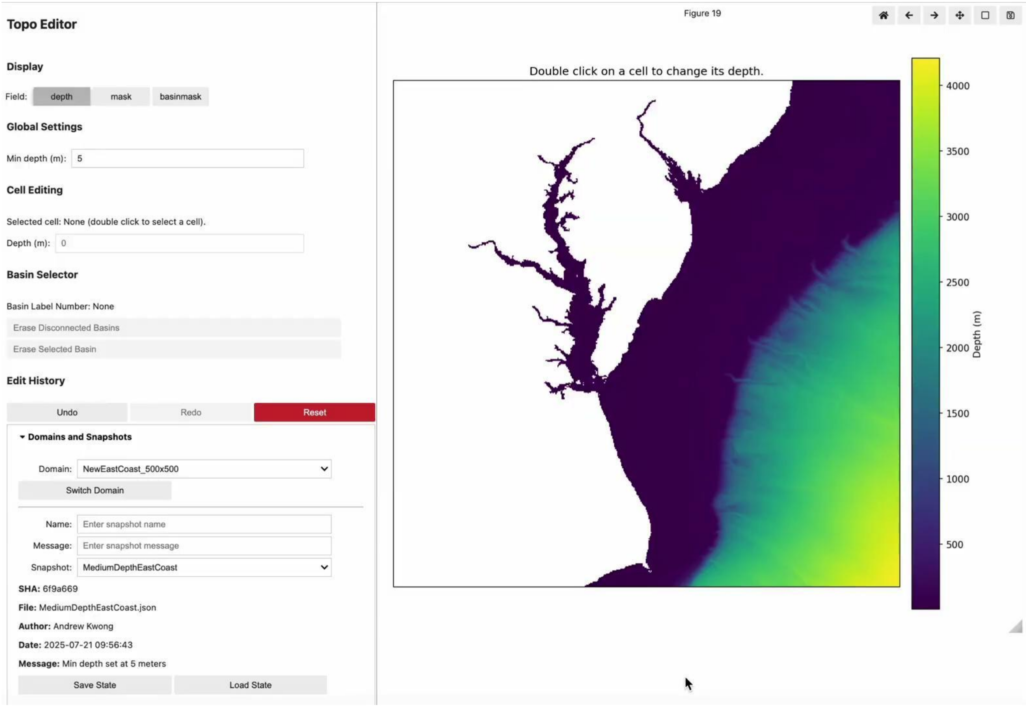
History

Version control →

Shareability

Editing topography is important for model tuning but tedious!

HISTORY AND PROVENANCE



Topo Editor

Display

Field: depth mask basinmask

Global Settings

Min depth (m): 5

Cell Editing

Selected cell: None (double click to select a cell).

Depth (m): 0

Basin Selector

Basin Label Number: None

Erase Disconnected Basins

Erase Selected Basin

Edit History

Undo Redo Reset

▾ Domains and Snapshots

Domain: NewEastCoast_500x500

Switch Domain

Name: Enter snapshot name

Message: Enter snapshot message

Snapshot: MediumDepthEastCoast

SHA: 6f9a669

File: MediumDepthEastCoast.json

Author: Andrew Kwong

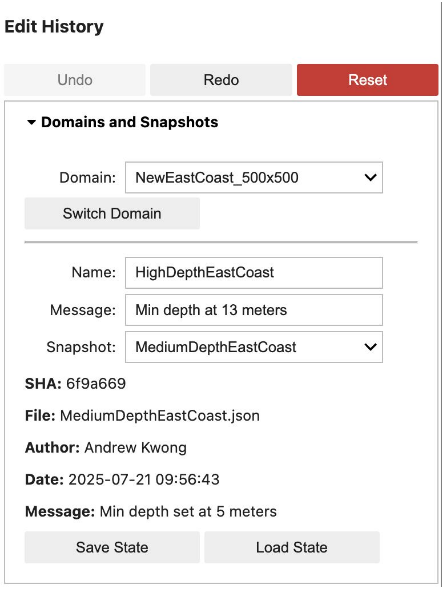
Date: 2025-07-21 09:56:43

Message: Min depth set at 5 meters

Save State Load State

Figure 19

Double click on a cell to change its depth.



Edit History

Undo Redo Reset

▾ Domains and Snapshots

Domain: NewEastCoast_500x500

Switch Domain

Name: HighDepthEastCoast

Message: Min depth at 13 meters

Snapshot: MediumDepthEastCoast

SHA: 6f9a669

File: MediumDepthEastCoast.json

Author: Andrew Kwong

Date: 2025-07-21 09:56:43

Message: Min depth set at 5 meters

Save State Load State

Topo Editor Edit History Section

Users now able to save and load snapshots across sessions, with a history **log** of modifications.

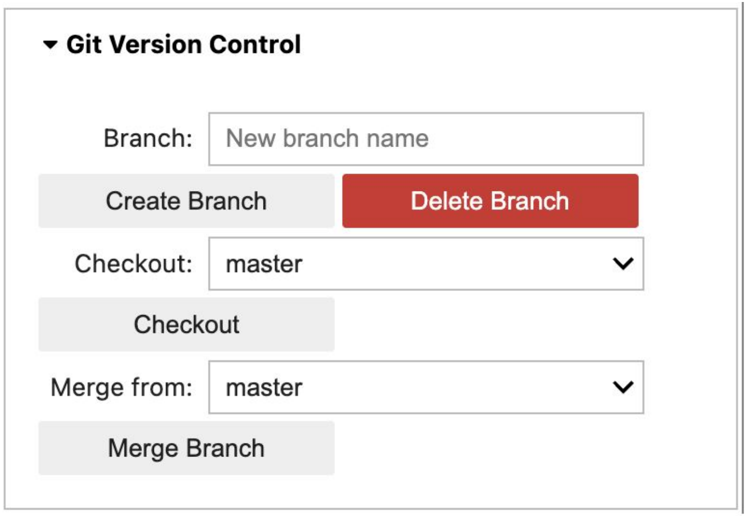
VERSION CONTROL INTEGRATION

With a history to log changes over time, how do we integrate version control?

We use **Git** to handle commits, branches, and checkouts in the Topo Editor.

This promotes data provenance and traceability!

Users can share Topo and Grid configurations through repositories.



▾ Git Version Control

Branch: New branch name

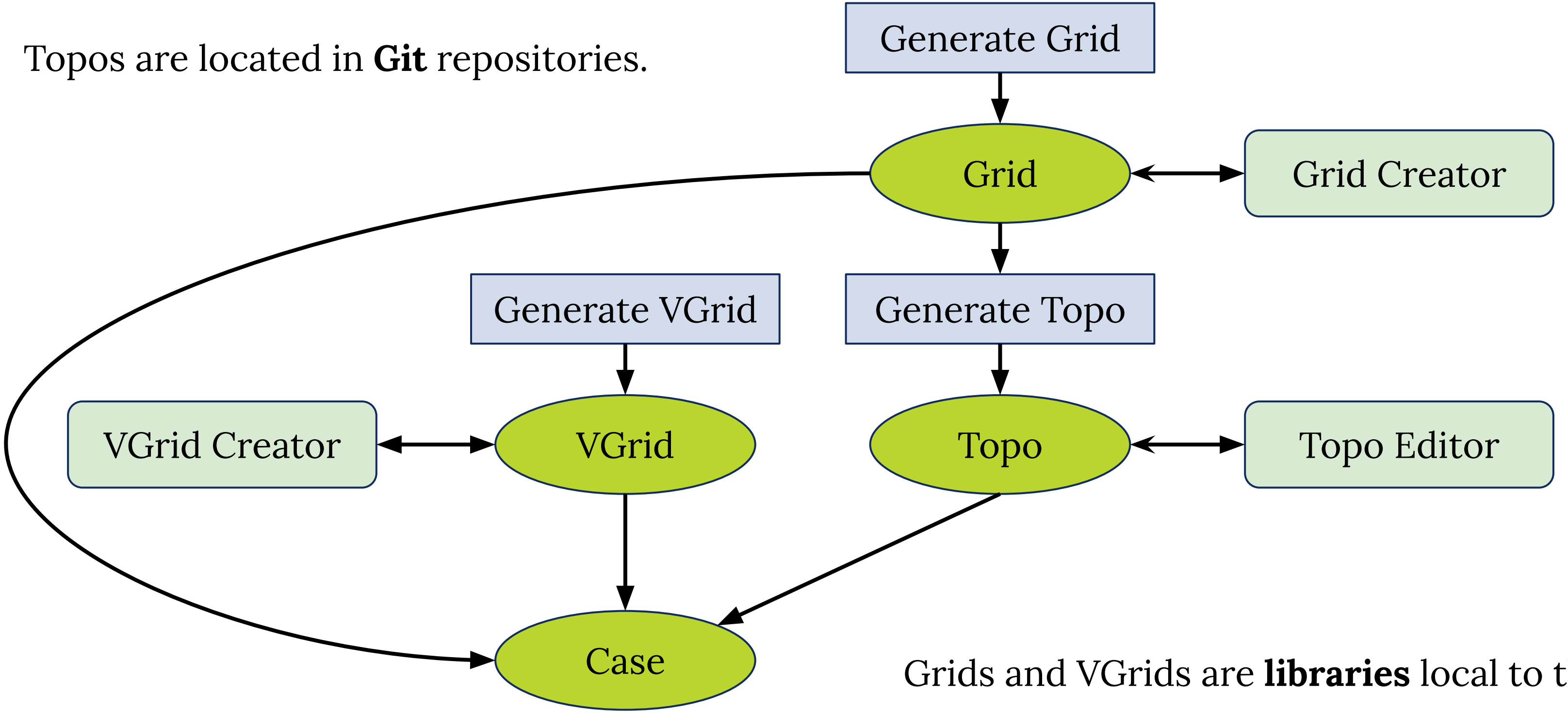
Checkout: master

Merge from: master

Topo Editor Version Control Section

STRUCTURE AND SHAREABILITY

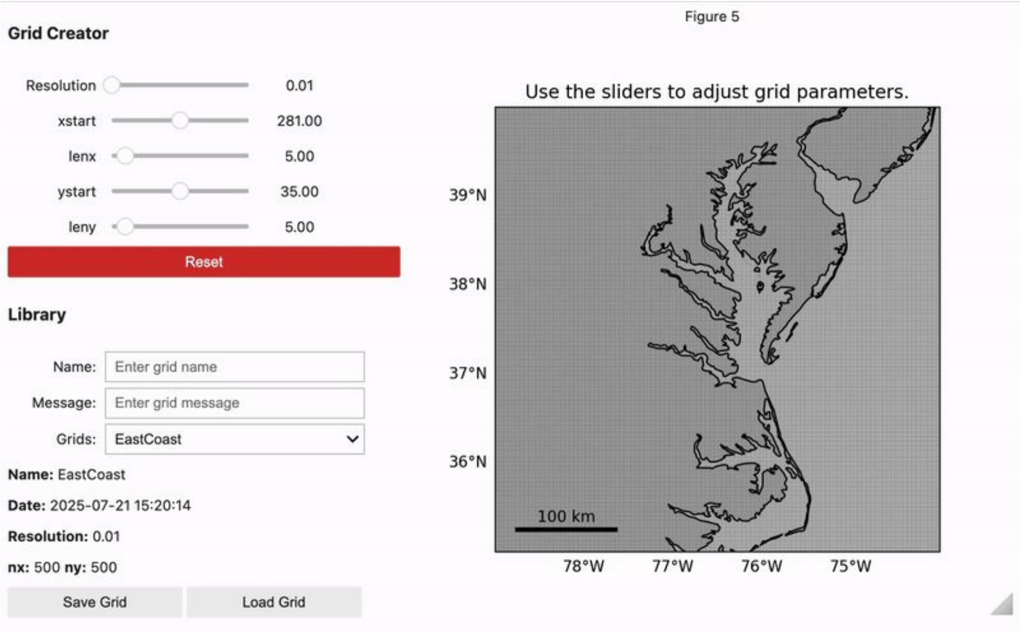
Topos are located in **Git** repositories.



Grids and VGrids are **libraries** local to the user.

OBJECT CONFIGURATORS

Grid Creator



Grid Creator

Resolution 0.01

xstart 281.00

lenx 5.00

ystart 35.00

leny 5.00

Reset

Library

Name: Enter grid name

Message: Enter grid message

Grids: EastCoast

Name: EastCoast

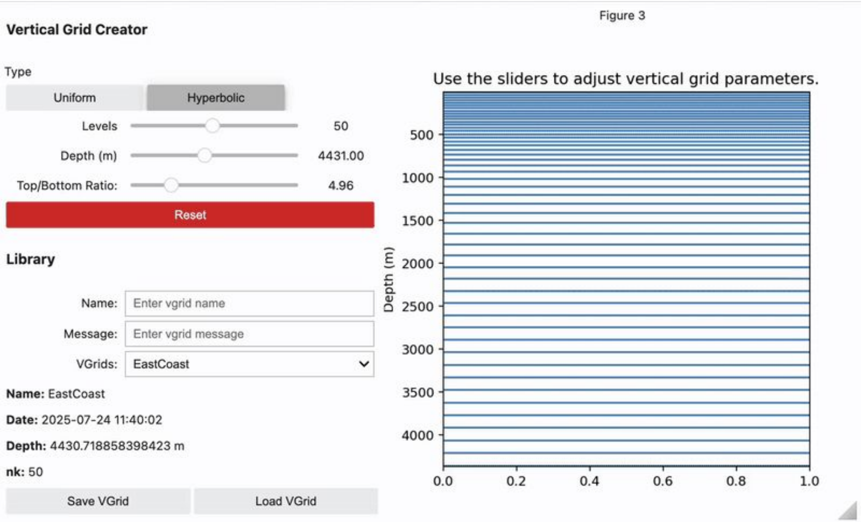
Date: 2025-07-21 15:20:14

Resolution: 0.01

nx: 500 **ny:** 500

Save Grid Load Grid

VGrid Creator



Vertical Grid Creator

Type

Uniform Hyperbolic

Levels 50

Depth (m) 4431.00

Top/Bottom Ratio: 4.96

Reset

Library

Name: Enter vgrid name

Message: Enter vgrid message

VGrids: EastCoast

Name: EastCoast

Date: 2025-07-24 11:40:02

Depth: 4430.718858398423 m

nk: 50

Save VGrid Load VGrid

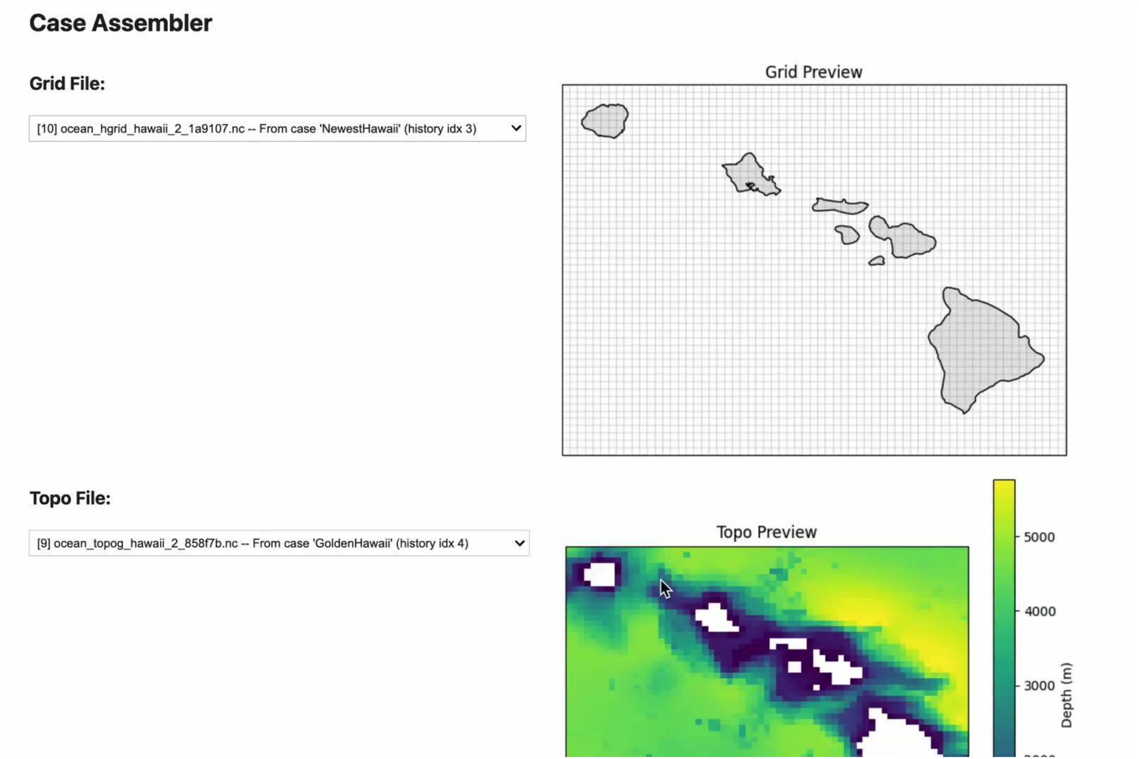
END-TO-END WORKFLOW

Final step: Add reproducibility to the preparation of forcing data.

Case history configurations are saved to a .json file.

We have everything we need to **build** and **run** a Case from history!

Case Assembler



Case Assembler

Grid File:

[10] ocean_hgrid_hawaii_2_1a9107.nc -- From case 'NewestHawaii' (history idx 3)

Topo File:

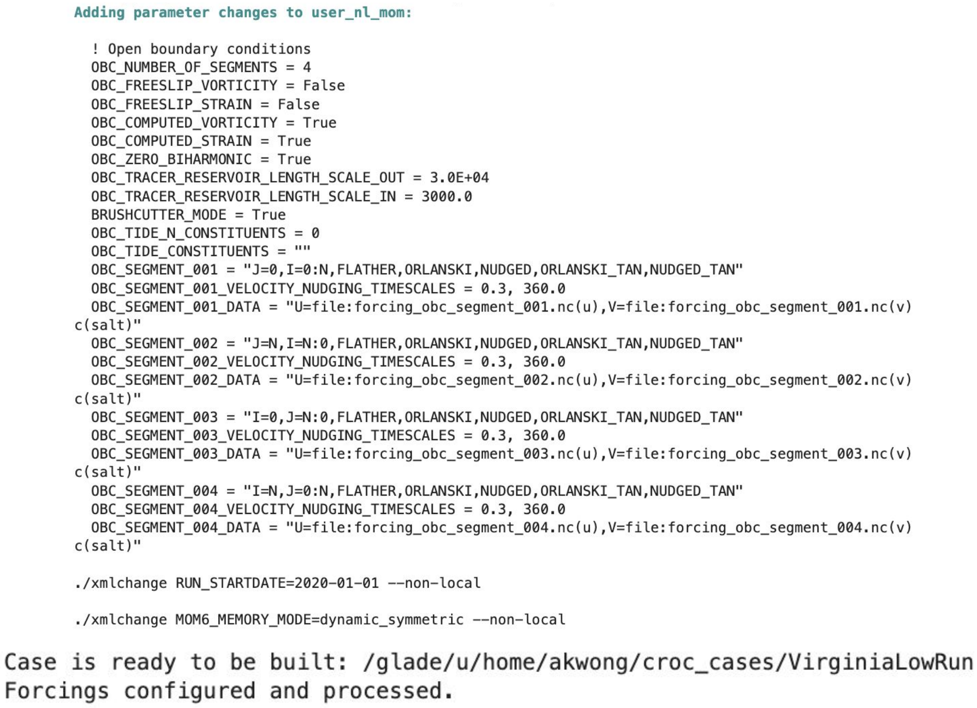
[9] ocean_topog_hawaii_2_858f7b.nc -- From case 'GoldenHawaii' (history idx 4)

END-TO-END WORKFLOW

Final step: Add reproducibility to the preparation of forcing data.

Case history configurations are saved to a .json file.

We have everything we need to **build** and **run** a Case from history!



```
Adding parameter changes to user_nl_mom:

  ! Open boundary conditions
  OBC_NUMBER_OF_SEGMENTS = 4
  OBC_FREESLIP_VORTICITY = False
  OBC_FREESLIP_STRAIN = False
  OBC_COMPUTED_VORTICITY = True
  OBC_COMPUTED_STRAIN = True
  OBC_ZERO_BIHARMONIC = True
  OBC_TRACER_RESERVOIR_LENGTH_SCALE_OUT = 3.0E+04
  OBC_TRACER_RESERVOIR_LENGTH_SCALE_IN = 3000.0
  BRUSHCUTTER_MODE = True
  OBC_TIDE_N_CONSTITUENTS = 0
  OBC_TIDE_CONSTITUENTS = ""
  OBC_SEGMENT_001 = "J=0,I=0:N,FLATHER,ORLANSKI,NUDGED,ORLANSKI_TAN,NUDGED_TAN"
  OBC_SEGMENT_001_VELOCITY_NUDGING_TIMESCALES = 0.3, 360.0
  OBC_SEGMENT_001_DATA = "U=file:forcing_obc_segment_001.nc(u),V=file:forcing_obc_segment_001.nc(v)
c(salt)"
  OBC_SEGMENT_002 = "J=N,I=N:0,FLATHER,ORLANSKI,NUDGED,ORLANSKI_TAN,NUDGED_TAN"
  OBC_SEGMENT_002_VELOCITY_NUDGING_TIMESCALES = 0.3, 360.0
  OBC_SEGMENT_002_DATA = "U=file:forcing_obc_segment_002.nc(u),V=file:forcing_obc_segment_002.nc(v)
c(salt)"
  OBC_SEGMENT_003 = "I=0,J=N:0,FLATHER,ORLANSKI,NUDGED,ORLANSKI_TAN,NUDGED_TAN"
  OBC_SEGMENT_003_VELOCITY_NUDGING_TIMESCALES = 0.3, 360.0
  OBC_SEGMENT_003_DATA = "U=file:forcing_obc_segment_003.nc(u),V=file:forcing_obc_segment_003.nc(v)
c(salt)"
  OBC_SEGMENT_004 = "I=N,J=0:N,FLATHER,ORLANSKI,NUDGED,ORLANSKI_TAN,NUDGED_TAN"
  OBC_SEGMENT_004_VELOCITY_NUDGING_TIMESCALES = 0.3, 360.0
  OBC_SEGMENT_004_DATA = "U=file:forcing_obc_segment_004.nc(u),V=file:forcing_obc_segment_004.nc(v)
c(salt)"

./xmlchange RUN_STARTDATE=2020-01-01 --non-local

./xmlchange MOM6_MEMORY_MODE=dynamic_symmetric --non-local

Case is ready to be built: /glade/u/home/akwong/croc_cases/VirginiaLowRun
Forcings configured and processed.
```

CONCLUSIONS

1. Reproducibility requires intention and infrastructure.

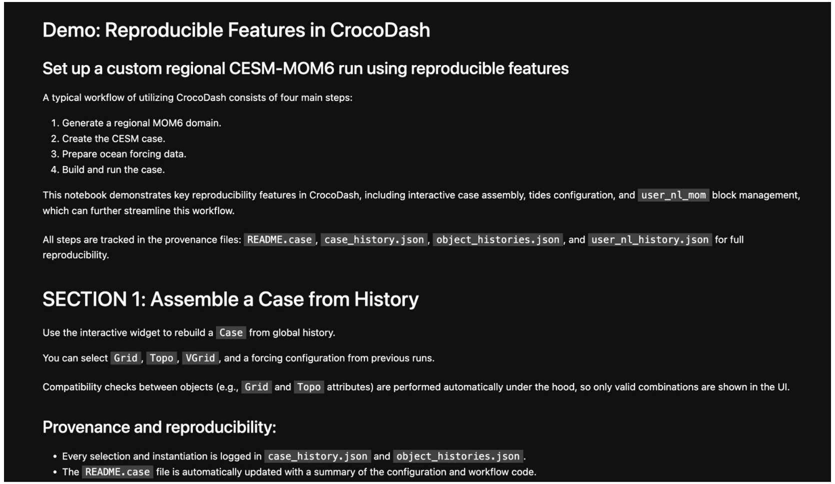
2. Modular design enables reusable modeling.

3. Good science begins with reproducibility.

Our work integrating modular configurators, version-controlled editing, and reproducible tools lays the foundation for rapid, reproducible Earth system modeling.

FUTURE WORK

Documentation



Demo: Reproducible Features in CrocoDash

Set up a custom regional CESM-MOM6 run using reproducible features

A typical workflow of utilizing CrocoDash consists of four main steps:

1. Generate a regional MOM6 domain.
2. Create the CESM case.
3. Prepare ocean forcing data.
4. Build and run the case.

This notebook demonstrates key reproducibility features in CrocoDash, including interactive case assembly, tides configuration, and `user_nl_mom` block management, which can further streamline this workflow.

All steps are tracked in the provenance files: `README.case`, `case_history.json`, `object_histories.json`, and `user_nl_history.json` for full reproducibility.

SECTION 1: Assemble a Case from History

Use the interactive widget to rebuild a `Case` from global history.

You can select `Grid`, `Topo`, `VGrid`, and a forcing configuration from previous runs.

Compatibility checks between objects (e.g., `Grid` and `Topo` attributes) are performed automatically under the hood, so only valid combinations are shown in the UI.

Provenance and reproducibility:

- Every selection and instantiation is logged in `case_history.json` and `object_histories.json`.
- The `README.case` file is automatically updated with a summary of the configuration and workflow code.

Create Jupyter notebooks focused on scientific reproducibility for regional MOM6 cases.

Testing

- Write unit tests for key components in the editors and in the Case Assembler.
- Develop a continuous integration (CI) pipeline for automated testing.

Extending Features

- Handle for other grid and edit types.
- Add to the reproducibility suite as CrocoDash grows (e.g., chlorophyll)!

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