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ROMS-Tools: Reproducible Preprocessing and Analysis for Regional Ocean Modeling with ROMS

Nora Loose [1], **Tom Nicholas** [2], **Scott Eilerman**[1], **Christopher McBride**[1], **Sam Maticka**[1], **Dafydd Stephenson**[1], **Scott Bachman**[1], **Pierre Damien**[3], **Ulla Heede**[1], **Alicia Karspeck**[1], **Matthew C. Long**[1], **M. Jeroen Molemaker**[3], and **Abigale Wyatt** [1]

1 [C]Worthy LLC, Boulder, CO, United States **2** Earthmover PBC **3** University of California, Los Angeles, CA, United States

DOI: 10.xxxxxx/draft

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Submitted: 01 January 1970
Published: unpublished

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Summary

The ocean regulates Earth's climate and sustains marine ecosystems by circulating and storing heat, carbon, oxygen, and nutrients, while exchanging heat and gases with the atmosphere. Scientists study these processes using ocean models, which simulate the ocean on a grid. **Regional ocean models** focus computational resources on a limited geographical area with fine grid spacing, and can resolve fine-scale phenomena such as mesoscale and submesoscale features, tidal dynamics, coastal currents, upwelling, and detailed biogeochemical (BGC) processes. A widely used regional ocean model is the **Regional Ocean Modeling System (ROMS)** (Shchepetkin & McWilliams, 2005). ROMS has been coupled to the Marine Biogeochemistry Library (MARBL) (Long et al., 2021; Molemaker & contributors, 2025a) to link physical and BGC processes. ROMS-MARBL supports research on environmental management, fisheries, regional climate impacts, and ocean-based carbon dioxide removal (CDR) strategies.

`ROMS-Tools` is a Python package that streamlines the **preparation and analysis of ROMS-MARBL simulations** by enabling users to generate regional grids, prepare model inputs, and analyze outputs efficiently. The package integrates with `xarray` (**?**) for labeled, multi-dimensional data handling, and supports large input and output datasets via parallel computation with `dask` (Dask Development Team, 2016), making workflows scalable from laptops to high-performance computing clusters. By providing a modern, user-friendly interface, `ROMS-Tools` lowers technical barriers, improves reproducibility, and allows scientists to focus on research rather than data preparation. The package is installable via Conda or PyPI and can be run interactively in Jupyter notebooks. Its modular design facilitates extension to new datasets.

Statement of Need

Regional ocean models are essential tools for research in marine ecosystems, climate dynamics, and ocean-based carbon dioxide removal (CDR). However, configuring a regional ocean model like ROMS-MARBL is technically demanding. Model setup requires initialization and time-dependent forcing from multiple oceanic and atmospheric datasets, drawn from multiple external sources in diverse formats. These global source datasets can span petabytes and must be subsetted, processed, and mapped onto the target model grid, producing 10–100 terabytes of input data for large regional domains. Generating these input files is time-consuming, error-prone, and difficult to reproduce. These challenges create a bottleneck for both new and experienced users, slow down science, and limit collaboration across groups.

Existing preprocessing tools within the ocean modeling ecosystem do not fully address these challenges for ROMS-MARBL. Legacy MATLAB-based scripts and packages such as `pyroms`

(Hedstrom & contributors, 2023) provide critical functionality but rely on low-level, manually coordinated steps that limit reproducibility, maintainability, and accessibility. In contrast, preprocessing frameworks developed for other ocean models (e.g., MOM6) cannot be directly applied to ROMS due to fundamental differences in grid geometry, vertical coordinates, and model input data requirements. As a result, ROMS-MARBL users lack a modern, integrated framework for reproducible model setup and analysis.

`ROMS-Tools` was developed to fill this gap. It is an open-source Python framework designed for researchers and practitioners who run ROMS or ROMS-MARBL regional ocean simulations, including users in physical oceanography, marine biogeochemistry, and ocean-based CDR applications. Current capabilities are fully compatible with UCLA-ROMS (Molemaker & contributors, 2025a, 2025b), with potential support for other ROMS implementations, such as Rutgers ROMS (Arango & contributors, 2024), in the future. The package provides high-level APIs that automate and standardize preprocessing workflows, manage complex model configuration state using explicit YAML-based specifications, and support reproducible simulation setup. By lowering technical barriers and improving transparency and reproducibility, `ROMS-Tools` enables more efficient model development, facilitates scientific collaboration, and supports applications such as verification of marine carbon removal strategies and carbon credit assessment.

State of the Field

Historically, setting up a regional ocean model required a patchwork of custom scripts and lab-specific workflows, resulting in error-prone and difficult-to-reproduce processes. Within the ROMS community, tools like `pyroms` (Hedstrom & contributors, 2023) addressed some of these issues by providing low-level Python utilities for preprocessing. However, `pyroms` has several limitations: installation is cumbersome due to Python/Fortran dependencies, the API is inconsistent, and documentation and tests are missing. The package does not support modern tools such as `xarray` and `dask`, nor reproducible workflows. Active development has ceased, and maintenance (including compatibility with newer Python versions) is no longer provided, making it very difficult to add new features, such as support for BGC tracers and CDR applications.

Tools from other modeling communities cannot be directly applied to ROMS because each model has distinct structural requirements and input conventions. For example, the `regional-mom6` package (Barnes et al., 2024), developed for regional configurations of the Modular Ocean Model v6 (MOM6) (Adcroft et al., 2019), cannot generate ROMS inputs. ROMS uses a terrain-following vertical coordinate system that requires specialized vertical regridding, whereas MOM6 accepts inputs on arbitrary depth levels and does not require vertical regridding at all. Within the broader ecosystem, `regional-mom6` is the closest analog to `ROMS-Tools`. Notably, the development cycles of `regional-mom6` and `ROMS-Tools` overlapped (`regional-mom6`: 2023–2024; `ROMS-Tools`: 2024–2025, based on public GitHub commits). Had the developers been aware of each other, a shared framework could potentially have been created, with model-specific adaptations layered on top. Adapting one framework to the other now would require extensive architectural changes.

Legacy MATLAB preprocessing scripts developed at UCLA (Molemaker, 2024) encapsulate decades of expertise in configuring regional ocean models, but require users to edit source code directly, making workflows error-prone, difficult to reproduce, and challenging to extend to new datasets or applications. `ROMS-Tools` provides a modern, open-source Python implementation of these scripts, retaining core algorithms while offering high-level APIs, automated intermediate steps, and explicit workflow state management via YAML. This object-oriented design improves reproducibility, reduces user errors, and supports extensibility, while leveraging modern Python tools such as `xarray` and `dask`. In some cases, `ROMS-Tools` diverges from the original MATLAB implementation to incorporate improved methods or better integrate with the Python ecosystem, creating a maintainable, scalable workflow for ROMS-MARBL simulations.

Overview of ROMS-Tools Functionality

`ROMS-Tools` provides a comprehensive workflow for generating, processing, and analyzing ROMS-MARBL model inputs and outputs, as detailed below.

Input Data and Preprocessing

`ROMS-Tools` generates the following input files for ROMS-MARBL:

1. **Model Grid**: Customizable, curvilinear, and orthogonal grid designed to maintain a nearly uniform horizontal resolution across the domain. The grid is rotatable to align with coastlines and features a terrain-following vertical coordinate.
2. **Bathymetry**: Derived from **SRTM15** (Tozer et al., 2019).
3. **Land Mask**: Inferred from coastlines provided by **Natural Earth** or the Global Self-consistent, Hierarchical, High-resolution Geography (**GSHHG**) Database (Wessel & Smith, 1996).
4. **Physical Ocean Conditions**: Initial and open boundary conditions for sea surface height, temperature, salinity, and velocities derived from the 1/12° Global Ocean Physics Reanalysis (**GLORYS**) (Lellouche et al., 2021).
5. **BGC Ocean Conditions**: Initial and open boundary conditions for dissolved inorganic carbon, alkalinity, and other biogeochemical tracers from Community Earth System Model (**CESM**) output (Yeager et al., 2022) or hybrid observational-model sources (Garcia et al., 2019; Huang et al., 2022; Lauvset et al., 2016; Yang et al., 2020; Yeager et al., 2022).
6. **Meteorological forcing**: Wind, radiation, precipitation, and air temperature/humidity processed from the global 1/4° ECMWF Reanalysis v5 (**ERA5**) (Hersbach et al., 2020) with optional corrections for radiation bias and coastal wind.
7. **BGC surface forcing**: Partial pressure of carbon dioxide, as well as iron, dust, and nitrogen deposition from **CESM** output (Yeager et al., 2022) or hybrid observational-model sources (Hamilton et al., 2022; Kok et al., 2021; Landschützer et al., 2016; Yeager et al., 2022).
8. **Tidal Forcing:** Tidal potential, elevation, and velocities derived from **TPXO** (Egbert & Erofeeva, 2002) including self-attraction and loading (SAL) corrections.
9. **River Forcing:** Freshwater runoff derived from **Dai & Trenberth** (Dai & Trenberth, 2002) or user-provided custom files.
10. **CDR Forcing**: User-defined interventions that inject BGC tracers at point sources or as larger-scale Gaussian perturbations to simulate CDR interventions. The CDR forcing is prescribed as volume and tracer fluxes (e.g., alkalinity for ocean alkalinity enhancement, iron for iron fertilization, or other BGC constituents). Users can control the magnitude, spatial footprint, and temporal evolution, allowing flexible representation of CDR interventions.

Some source datasets are accessed automatically by `ROMS-Tools`, including Natural Earth, Dai & Trenberth runoff, and ERA5 meteorology, while users must manually download SRTM15, GSHHG, GLORYS, the BGC datasets, and TPXO tidal files. Although these are the datasets currently supported, the modular design of `ROMS-Tools` makes it straightforward to add new source datasets in the future.

To generate the model inputs, `ROMS-Tools` automates several intermediate processing steps, including:

- **Bathymetry processing**: The bathymetry is smoothed in two stages, first across the entire model domain and then locally in areas with steep slopes, to ensure local steepness ratios do not exceed a prescribed threshold in order to reduce pressure-gradient errors. A minimum depth is enforced to prevent water levels from becoming negative during large tidal excursions.

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- **Mask definition**: The land-sea mask is generated by comparing the ROMS grid's horizontal coordinates with a coastline dataset using the `regionmask` package (Hauser et al., 2024). Enclosed basins are subsequently filled with land.
- **Land value handling**: Land values are filled via an algebraic multigrid method using `pyamg` (Bell et al., 2023) prior to horizontal regridding. This extends ocean values into land areas to reconcile discrepancies between source data and ROMS land masks, ensuring that no NaNs or land-originating values contaminate ocean grid cells.
- **Regridding**: Ocean and atmospheric fields are horizontally and vertically regridded from standard latitude-longitude-depth grids to the model's curvilinear grid with a terrain-following vertical coordinate using `xarray` (Hoyer & Hamman, 2017) and `xgcm` (Busecke & contributors, 2025). Velocities are rotated to align with the curvilinear ROMS grid.
- **Longitude conventions**: `ROMS-Tools` handles differences in longitude conventions, converting between [-180°, 180°] and [0°, 360°] as needed.
- **River locations**: Rivers that fall within the model domain are automatically identified and relocated to the nearest coastal grid cell. Rivers that need to be shifted manually or span multiple cells can be configured by the user.
- **Data streaming**: ERA5 atmospheric data can be accessed directly from the cloud, removing the need for users to pre-download large datasets locally. Similar streaming capabilities may be implemented for other datasets in the future.

Users can quickly design and visualize regional grids and inspect all input fields with built-in plotting utilities. An example of surface initial conditions generated for a California Current System simulation at 5 km horizontal grid spacing is shown in Figure 1.

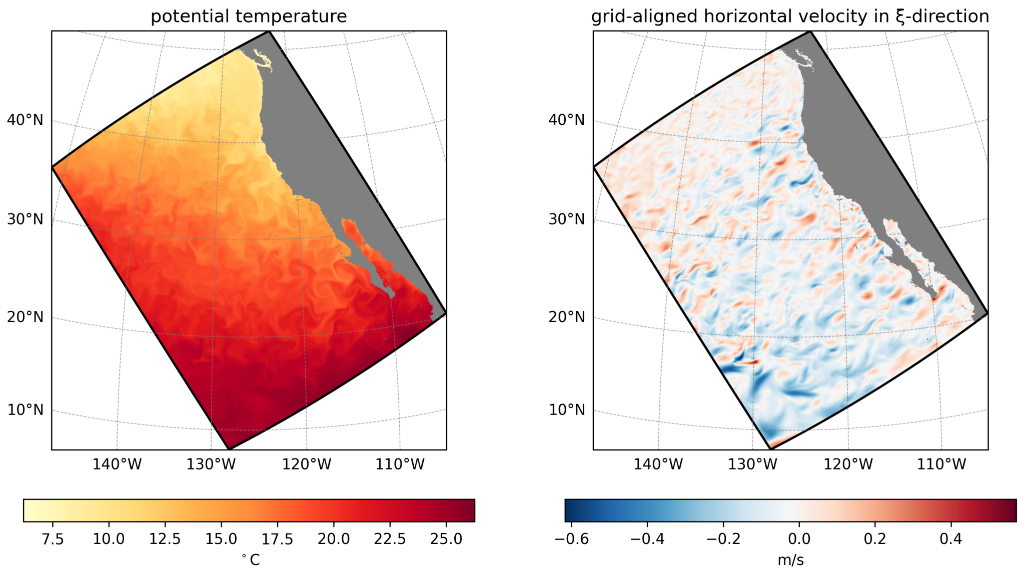

Figure 1: Surface initial conditions for the California Current System created with `ROMS-Tools` from GLORYS. Left: potential temperature. Right: grid-aligned horizontal velocity in ξ-direction. Shown for January 1, 2000.

Software Design

`ROMS-Tools` is designed to balance **ease of use, flexibility, reproducibility, and scalability** by combining high-level user interfaces with a modular, extensible architecture.

Lessons from MATLAB Tools

The legacy MATLAB preprocessing scripts were powerful but required users to edit source code directly to configure simulations. This workflow led to frequent errors for new users, made it difficult to track completed steps, and limited reproducibility. `ROMS-Tools` addresses these issues with **high-level API calls**, automated error-prone steps, and explicit workflow state management via YAML.

Design Trade-Offs

A central design trade-off in `ROMS-Tools` is between **user control** and **automation**. Rather than enforcing a fixed workflow, the package exposes key choices such as physical options (e.g., corrections for radiation or wind), interpolation and fill methods, and computational backends. This approach contrasts with opinionated frameworks that fix defaults and directory structures to maximize automation. While users must make explicit decisions, some steps remain automated to prevent errors. For example, bathymetry smoothing is applied automatically using a fixed, non-tunable parameter, since insufficient or omitted smoothing can crash simulations due to pressure gradient errors. This design choice directly addresses issues new users faced in the MATLAB scripts, and balances **flexibility** and **safety**, enabling transparent experimentation without exposing users to avoidable pitfalls.

Another key design consideration is balancing **modular, incremental workflow steps** with **reproducibility**. `ROMS-Tools` organizes tasks (such as creating `InitialConditions`, `BoundaryForcing`, and `SurfaceForcing`) into small, composable components that can be executed, saved, and revisited independently, rather than following a monolithic, fixed workflow. All components depend on the `Grid`, but once it is created, the remaining objects are independent. This modular approach avoids unnecessary recomputation when only some inputs change but requires careful tracking of workflow state. To ensure reproducibility, all configuration choices are stored in compact, text-based YAML files. These files are version-controllable, easy to share, and eliminate the need to transfer large model input NetCDF datasets. By explicitly tracking workflow state, this design overcomes a key limitation of the MATLAB scripts and helps users manage experiments more reliably.

Architecture

At the user-facing level, `ROMS-Tools` provides high-level objects such as `Grid`, `InitialConditions`, and `BoundaryForcing`. Each object exposes a consistent interface (`.ds`, `.plot()`, `.save()`, `.to_yaml()`), allowing users to call the same methods in sequence and inspect attributes that are always present. This design reduces cognitive overhead, makes workflows predictable, and removes the need for new users to edit raw scripts or manually track intermediate files, as was required with the MATLAB tools.

Internally, `ROMS-Tools` follows a **layered, modular architecture**. Low-level classes (`LatLonDataset`, `ROMSDataset`) handle data ingestion and preprocessing, including common operations such as subdomain selection and lateral land filling. Source-specific datasets (e.g., `ERA5Dataset`, `GLORYSDataset`, `SRTMDataset`) inherit from these base classes and encode dataset-specific conventions like variable names, coordinates, and masking. Adding support for a new data source typically requires only a small subclass to define variable mappings while reusing existing logic, minimizing changes to the core code. High-level classes (`Grid`, `InitialConditions`, `BoundaryForcing`) build on these low-level datasets to produce ready-to-use modeling inputs, performing tasks such as regridding and final assembly. This layered design enhances **extensibility and maintainability**, avoiding the pitfalls of the monolithic MATLAB scripts.

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Computational and Data Model Choices

`ROMS-Tools` is built on `xarray`, which provides a clear, consistent interface for exploring and inspecting labeled, multi-dimensional geophysical datasets. Users can take advantage of `xarray`'s intuitive indexing, plotting, and metadata handling. Optional `dask` support allows workflows to scale from laptops to HPC systems, enabling parallel and out-of-core computation for very large input and output datasets. By combining modern Python tools with a user-friendly interface, `ROMS-Tools` addresses the usability challenges that hampered new users in the MATLAB-based workflow.

Research Impact Statement

`ROMS-Tools` is used by two primary research communities. First, regional ocean modelers use it to generate reproducible input datasets for ROMS simulations; external users include researchers at **PNNL**, **WHOI**, and **UCLA**. Second, researchers in the ocean-based carbon dioxide removal (CDR) community use `ROMS-Tools` to configure reproducible ROMS–MARBL simulations of climate intervention scenarios, with adopters including **[C]Worthy**, **Carbon to Sea**, **Ebb Carbon**, and **SCCWRP**. All of these groups have contacted the developers directly or engaged with the project through GitHub or offline discussions. Several manuscripts from these communities are currently in preparation.

Beyond standalone use, ROMS-Tools is integrated into broader scientific workflows, including C-Star (Stephenson & contributors, 2025), an open-source platform that provides scientifically credible monitoring, reporting, and verification (MRV) for the emerging marine carbon market.

Additional evidence of community uptake comes from public usage metrics. At the time of writing, the GitHub repository shows **119 unique cloners in the past 14 days**, with stars from users at institutions including the University of Waikato, NCAR, University of Maryland, National Oceanography Centre, McGill University, UC Santa Cruz, and others. Distribution statistics indicate **over 3,100 conda-forge downloads in the past six months**, including **68 downloads of the most recent release** (`v3.3.0`), and **more than 48,000 total PyPI downloads**. PyPI counts include automated continuous integration (CI) usage by `ROMS-Tools`, in addition to direct user installations. In contrast, conda-forge downloads of `v3.3.0` reflect exclusively human-initiated installs, as C-Star's CI workflows currently pin pre-`v3.3.0` releases of `ROMS-Tools`.

Postprocessing and Analysis

`ROMS-Tools` supports postprocessing and analysis of ROMS-MARBL output, including regridding from the native curvilinear, terrain-following grid to a standard latitude-longitude-depth grid using `xesmf` (Zhuang et al., 2023), with built-in plotting for both grid types. The analysis layer also includes specialized utilities for evaluating carbon dioxide removal (CDR) interventions, such as generating carbon uptake and efficiency curves.

AI Usage Disclosure

Generative AI tools were used to help write docstrings, develop tests, and improve the clarity and readability of both the ROMS-Tools documentation and manuscript text. All AI-assisted content was reviewed and verified by the authors for technical accuracy and correctness.

Acknowledgements

Development of `ROMS-Tools` has been supported by ARPA-E (DE-AR0001838) and philanthropic donations to [C]Worthy from the Grantham Foundation for the Environment,

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the Chan Zuckerberg Initiative, Founders Pledge, and the Ocean Resilience Climate Alliance.

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