ROMS-Tools: Reproducible Preprocessing and Analysis for ROMS Simulations

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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 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, resolving 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.

Configuring a regional ocean model like ROMS-MARBL is technically challenging. Setting up a model requires initializing and forcing it with oceanic and atmospheric data from multiple external sources in diverse formats, which can reach several petabytes for global datasets. These data must be subsetted, processed, and mapped onto the target domain's geometry, producing input datasets of 10–100 terabytes for large regional models. Generating these input files is time-consuming, error-prone, and hard to reproduce, creating a bottleneck for both new and experienced users. The Python package `ROMS-Tools` addresses this challenge by providing efficient, dask-backed (Dask Development Team, 2016), user-friendly tools that can be installed via Conda or PyPI and run interactively from Jupyter notebooks. It supports creating regional grids, preprocessing all required model inputs, and postprocessing and analysis. Current capabilities are fully compatible with UCLA-ROMS (Molemaker & contributors, 2025a, 2025b), with potential support for other ROMS versions, such as Rutgers ROMS (Arango & contributors, 2024), in the future.

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, designed to simulate CDR interventions. The CDR forcing provides an external forcing term prescribed as volume and tracer fluxes (e.g., alkalinity for ocean alkalinity enhancement, iron for iron fertilization, or other BGC constituents). Users can specify the magnitude, spatial footprint, and time dependence of the forcing, enabling flexible representation of CDR interventions.

Some source datasets are accessed automatically by the package, 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 package's modular design makes it straightforward to add new sources 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.
- **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 resolve discrepancies between source data and ROMS land masks, preventing land-originating values from appearing in ocean 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). Optional sea surface height corrections can be applied, and 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.

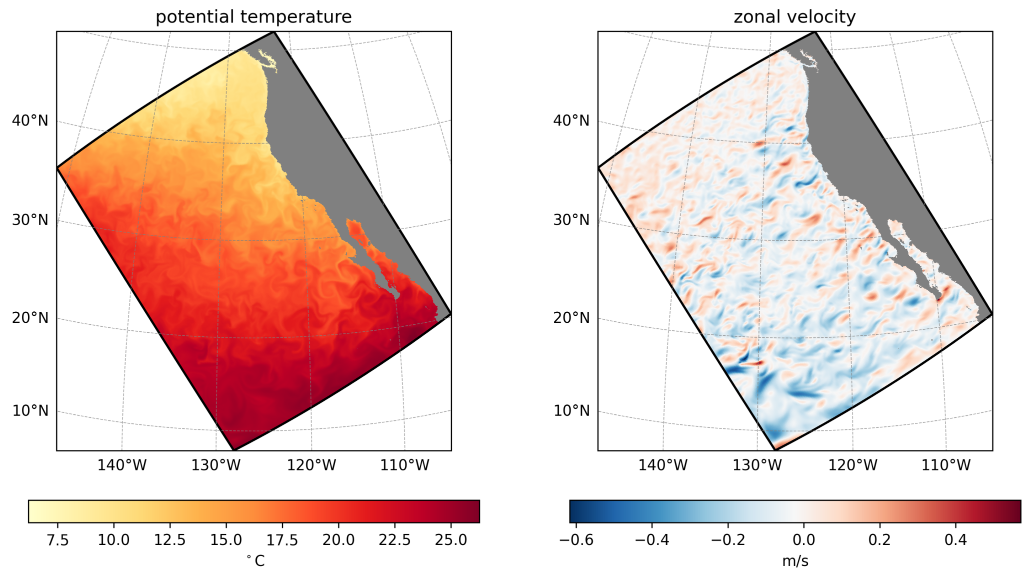

Figure 1: Surface initial conditions for the California Current System created with `ROMS-Tools` from GLORYS. Left: potential temperature. Right: zonal velocity. Shown for January 1, 2000.

Postprocessing and Analysis

`ROMS-Tools` provides tools for postprocessing and analyzing 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) and built-in plotting on both grids. The analysis layer also includes specialized utilities for evaluating carbon dioxide removal (CDR) interventions, such as generating carbon uptake and efficiency curves.

Statement of Need

Setting up a regional ocean model is a major technical undertaking. Traditionally, this work relied on a patchwork of custom scripts and lab-specific workflows, which can be time-consuming, error-prone, and difficult to reproduce. These challenges slow down science, create a steep barrier to entry for new researchers, and limit collaboration across groups.

Within the ROMS community, the preprocessing landscape has been shaped by tools like `pyroms` (Hedstrom & contributors, 2023). While providing valuable low-level utilities, `pyroms` presents challenges for new users: installation is cumbersome due to Python/Fortran dependencies, the API is inconsistent, documentation is limited, and it lacks tests, CI, and support for modern Python tools like `xarray` and `dask`. Since active development has largely ceased, its suitability for new projects, such as CDR simulations, is limited.

Tools from other modeling communities cannot simply be adopted, since each ocean model has distinct structural requirements. For example, the new `regional-mom6` package (Barnes et al., 2024), developed for the Modular Ocean Model v6 (MOM6) (Adcroft et al., 2019), cannot be used to generate ROMS inputs, because ROMS employs a terrain-following vertical coordinate system that requires a specialized vertical regridding approach, whereas MOM6 accepts inputs on arbitrary depth levels and does not require vertical regridding at all. Several other differences further prevent cross-compatibility. Together, these limitations underscored the need for a modern, maintainable, and reproducible tool designed specifically for ROMS.[1]

`ROMS-Tools` was developed to meet this need. It draws on the legacy of the MATLAB preprocessing scripts developed at UCLA (Molemaker, 2024), which encapsulate decades of expertise in configuring regional ocean model inputs. While many of the core algorithms and design principles are retained, `ROMS-Tools` provides an open-source Python implementation of these MATLAB tools using an object-oriented programming paradigm. This implementation enables a modernized workflow driven by high-level user API calls, enhancing reproducibility, reducing the potential for user errors, and supporting extensibility for additional features, forcing datasets, and use cases. In some cases, `ROMS-Tools` diverges from the MATLAB implementation to take advantage of new methods or better integration with the modern Python ecosystem. By streamlining input generation and analysis, `ROMS-Tools` reduces technical overhead, lowers the barrier to entry, and enables scientists to focus on research rather than data preparation.

Software Design

`ROMS-Tools` is designed to balance **ease of use, flexibility, reproducibility, and scalability** in regional ocean modeling workflows, providing both high-level user interfaces and a modular, extensible architecture that supports efficient data handling, customizable workflows, and scalable computation.

Design Trade-Offs

A central design trade-off in `ROMS-Tools` is between **automation** and **user control**. Rather than enforcing a fixed workflow, the package exposes key choices, such as physical options (e.g., radiation or wind corrections), interpolation and fill methods, and computational backends. This contrasts with more opinionated frameworks that fix defaults and directory structures to maximize automation. While users make explicit decisions, some steps remain automated to prevent errors; for example, bathymetry smoothing is applied automatically with a non-tunable parameter, since overly small smoothing factors could produce rough bathymetry and crash simulations. This approach balances flexibility and safety, enabling transparent experimentation without exposing users to avoidable pitfalls.

Another key trade-off is between **monolithic workflows** and **incremental, modular steps**. `ROMS-Tools` uses small, composable components, such as generating initial conditions, boundary forcing, and surface forcing. Each component can be executed, saved, and revisited independently. This avoids unnecessary recomputation when only some inputs change. To ensure reproducibility despite a modular workflow, configuration choices are stored in compact, text-based YAML files. These files are version-controllable, easy to share, and remove the need to transfer large model input NetCDF datasets.

Architecture and Rationale

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()`), so users can always call the same methods in sequence or inspect attributes that are guaranteed to exist. This object-oriented design reduces cognitive overhead and makes workflows predictable and easy to follow.

[1] In the future, packages like ROMS-Tools and regional-mom6 could share a common backbone, with model-specific adaptations layered on top.

Internally, `ROMS-Tools` uses a **layered, modular architecture**. Abstract base classes (`LatLonDataset`, `ROMSDataset`) handle data ingestion and preprocessing. Source-specific datasets (e.g., `ERA5Dataset`, `GLORYSDataset`, `SRTMDataset`) inherit from these base classes and encode dataset-specific conventions, such as variable names, coordinates, and masking. Common operations, like subdomain selection and lateral filling, are implemented once and reused across datasets. Adding a new data source usually requires only a small subclass to define variable mappings while reusing the existing subsetting, filling, regridding, and I/O logic. This approach keeps changes to the core code minimal.

Computational and Data Model Choices

`ROMS-Tools` is built on `xarray`, which lets users take advantage of its clear, consistent interface for exploring and inspecting datasets. The package integrates seamlessly with the broader Pangeo ecosystem. Optional `dask` support (Dask Development Team, 2016) allows workflows to scale from a laptop to HPC systems, enabling parallel and out-of-core computation for very large input and output datasets.

Research Impact Statement

`ROMS-Tools` serves two primary user communities. First, ocean modelers developing new regional domains rely on it to generate input datasets for ROMS simulations. External users in this category include researchers at **PNNL**, **WHOI**, **UCLA**, and in **New Zealand and Australia**. Second, researchers in the ocean-based carbon dioxide removal (CDR) community use `ROMS-Tools` to set up reproducible ROMS-MARBL simulations of climate intervention scenarios, with adopters such as **[C]Worthy**, **Carbon to Sea**, **Ebb Carbon**, and **SCCWRP**. All of these users have contacted the developers directly or consulted offline regarding their use of the package.

Broader engagement is evident from GitHub stars, with users from institutions including the University of Waikato, NCAR, University of Maryland, National Oceanography Centre, Fathom Science, McGill University, Gwangju Institute of Science and Technology, UC Santa Cruz, RedLine Performance Solutions, and Submarine.

`ROMS-Tools` is also integrated into broader workflows, including **C-Star**, an open-source platform to provide scientifically credible monitoring, reporting, and verification (MRV) for the emerging marine carbon market.

AI usage disclosure

Generative AI tools were used to assist with writing docstrings and developing tests for the `ROMS-Tools` software, to improve the clarity and readability of the documentation, and to shorten and edit portions of the manuscript text. All AI-assisted content was reviewed and verified by the authors for technical accuracy and correctness.

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