AIBECS.jl: A tool for exploring global marine biogeochemical cycles.

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Summary

The ocean transports, mixes, and transforms chemical constituents on a multitude of time and length scales. Observations and models are both essential for making sense of this complex system. However, the days of just publishing data without any quantitative modelling are over, increasing pressure on sea-going oceanographers that are expected to be proficient in the use of biogeochemical models. And while the simplest of these models consist of only a few boxes (e.g., the two-box model of Archer et al., 2000), with solutions that are easily obtained by hand or on a simple desktop computer, the most advanced models have high-resolution three-dimensional meshes that require high-performance computing (HPC) clusters and a considerable amount of computational-science expertise (e.g., the MITgcm, Campin et al., 2021). A high barrier to entry for modelling in oceanography hinders advances in the field. AIBECS.jl (Pasquier, 2021) is a JuliaOcean-affiliated package written in Julia (Bezanson et al., 2017), which aims to lower this barrier by providing an easy-to-use, open-source, and modular framework for simulating global marine tracers in steady-state and biogeochemical parameter fitting.

A conceptual model of the cycle of any marine tracer essentially requires two components. (i) A model of how the tracer is transported (be it the ocean currents and eddies, gravitational settling, or a combination of those), and (ii) a model of the local sources and sinks at any location. AIBECS.jl is built on this concept and allows users to build numerical models of marine tracers by selecting a circulation and/or vertical transport of the tracer with particles and local sources and sinks. Tools for generating the steady-state equations, solving them, and then diagnosing and plotting the simulated tracers are also provided, either directly by AIBECS.jl, by its dependencies, or by satellite packages in the AIBECS and Julia ecosystem.

Box (1979) has remarked that, by definition, all models are wrong because they make simplifying assumptions. These assumptions can give rise to model parameters that can capture fundamental characteristics of the system. Once the model of the cycle of a marine tracer is implemented, it is thus natural to try to estimate biogeochemical parameters by minimizing model–observation mismatches, which may improves the skill of the model. Parameter optimization is generally more efficiently performed when first and second derivatives are available, and these derivatives can also be used to estimate parameter sensitivity (Thacker, 1989). AIBECS.jl was designed with parameter fitting in mind and provides, along with satellite packages, tools for generating first- and second-order derivatives automatically and efficiently.

The AIBECS.jl package builds on the vision of the AWESOME OCIM (A Working Environment for Simulating Ocean Movement and Elemental cycling within the Ocean Circulation Inverse

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Model, or AO, John et al., 2020), which was designed to make three-dimensional element-cycling models more broadly accessible. Written in Julia — chosen for of its combined expressive power and efficiency and offering a truly open-source solution — the AIBECS.jl framework improves on the AO on a number of fronts to target education and research. Simple AIBECS.jl simulations can be produced in minutes in interactive notebooks while resource-hungry projects, e.g., for optimizing models with multiple tracers interacting nonlinearly within a high-resolution mesh, can be easily version-controlled, hosted, and run on HPC clusters.

Through a simple user interface, AIBECS.jl provides access to a variety of steady-state ocean circulation models. These currently include the Ocean Circulation Inverse Model (OCIM) v0.1 (Primeau et al., 2013), v1.0 (DeVries, 2014; DeVries & Primeau, 2011), and v2.0 (DeVries & Holzer, 2019), and the MITgcm-built Ocean Comprehensible Atlas (OCCA) ocean-state estimate model (Forget, 2010), of which the downloads are handled by the DataDeps.jl package (White et al., 2018, 2019). AIBECS.jl also offers classic two-box and three-box models (Archer et al., 2000; Sarmiento & Gruber, 2006). The OceanGrids.jl package, on which AIBECS depends, provides the underlying grid configuration types as well as regridding and interpolating routines. Swapping the underlying circulation model and grid requires a single-line-of-code change, facilitating intercomparison projects. As new circulation models that are represented in matrix form are made publicly available, they will be added to the collection. These could include past- and future-ocean circulation models, for paleoceanographic or climate-change studies, for example.

AIBECS.jl also provides extra functionality to facilitate the generation of numerical models. Tooling to simulate gravitational settling of tracers with non-buoyant particles is provided by the `transportoperator` function. In addition, AIBECS provides access to a number of predefined fields that can be used to generate source and sink processes. Fine-resolution (1-arc-minute) topography from the ETOPO1 dataset (Amante & Eakins, 2009) can be used for a refined interception of particulate fluxes by subgrid topographic features not captured by coarser circulation models. For aeolian deposition, AIBECS.jl includes aerosol-type- and region-of-origin-partitioned dust deposition fields (Chien et al., 2016; Kok et al., 2021). Datasets for global river discharge (Dai, 2017; Dai & Trenberth, 2002) and surface groundwater discharge (Luijendijk et al., 2019, 2020) are included. For hydrothermal-sourced tracers, the helium fluxes from the Earth's mantle computed with the OCIM v1.0 and v2.0 are available when loading the corresponding circulation models (DeVries, 2014; DeVries & Holzer, 2019). AIBECS.jl also provides access to the data included with the AWESOME OCIM framework (John et al., 2020), namely data from the Global Ocean Data Analysis Project (GLODAP, Lauvset et al., 2016; Olsen et al., 2016), P-cycling modelled fields from Weber et al. (2018), nepheloid layers (Gardner, Richardson, & Mishonov, 2018; Gardner, Richardson, Mishonov, & Biscaye, 2018; Taburet et al., 2019), as well as other data already present within AIBECS or satellite packages. Also useful to global biogeochemistry modelling are data from the World Ocean Atlas (Garcia et al., 2018) that can be downloaded, assisted by external package WorldOceanAtlasTools.jl (Pasquier, 2019). Similarly, GEOTRACES data (Schlitzer et al., 2018) can be handled by the GEOTRACES.jl package (although GEOTRACES requires manual download of the data). More advanced usage such as optimization is facilitated by the F1Method.jl package (Pasquier, 2020), which provides efficient gradient and Hessian computations of objective functions defined through AIBECS.jl, which can then be directly fed to optimization routines from, e.g., the Optim.jl package (Mogensen & Riseth, 2018). Finally, plotting recipes for the Plots.jl package (Breloff, 2021), are available.

Internally, AIBECS.jl uses a quasi-Newton solver (Kelley, 2003) translated from MATLAB to Julia and tailored to the context of marine tracers to solve/simulate tracers. AIBECS uses forward-mode auto-differentiation from the ForwardDiff.jl package (Revels et al., 2016) for the nonlinear parts of the system of ordinary differential equations to generate the Jacobian required for the solver. Metadata such as units and prior distributions can be attached to model parameters, which are handled with the help of the UnPack.jl, FieldMetadata.jl, Flatten.jl, DataFrames.jl, Distributions.jl (Besançon et al., 2021; Lin et al., 2019), Unitful.jl, and

95 Bijectors.jl dependencies.

96 The AIBECS.jl package is registered with Julia's default package registry (GENERAL), such
97 that installation takes a single line of code from within Julia. The package documentation,
98 which is built through continuous integration (CI), includes tutorials and how-to guides that
99 are both available online for consultation and as runnable Jupyter notebooks. Continuous
100 integration through GitHub actions also includes a fairly complete suite of tests.

Statement of need

102 Pioneered by Schlitzer (1993) to study the ocean circulation using ventilation tracers such
103 as radiocarbon (see also Schlitzer, 2000), the low computational costs of steady-state cir-
104 culation models allow for efficient optimization and inference/estimation of biogeochemical
105 parameters. Today, despite reduced resolution and steady-state assumption, data-constrained
106 matrix-transport models such as the OCIM are at the forefront of oceanographic research.
107 This is evidenced for example by the growing number of high-profile studies that use such
108 models for parameter estimation published in recent years (e.g., DeVries et al., 2017, 2012,
109 2013; DeVries, 2014; DeVries & Deutsch, 2014; DeVries & Weber, 2017; Roshan & DeVries,
110 2017; Teng et al., 2014; Wang et al., 2019; Weber et al., 2016; Weber & Deutsch, 2010).
111 However, although the steady-state assumption and matrix representation simplify the simu-
112 lation of tracers compared to traditional Ocean General Circulation Models (OGCMs), most
113 studies that employ a steady-state matrix representation of marine cycling remain difficult to
114 reproduce without significant computer-science and modelling expertise because they are built
115 on private implementations. Comparisons between different circulation models are moreover
116 complicated by the lack of standardization across models.

117 Hence, there is a need to facilitate the use of steady-state ocean-circulation models by provid-
118 ing: (i) an integrated framework for handling a number of different ocean-circulation models
119 with tools for swapping circulations (including interpolating from one model grid to another),
120 (ii) a user-friendly interface for translating mathematical models of biogeochemical cycles into
121 the corresponding code (e.g., for sources, sinks, and vertical transport of tracers), and (iii)
122 solvers for efficient simulations, optimization, diagnosis, and statistical analysis.

123 AIBECS.jl provides a free, open-source, unified framework for biogeochemical-tracer-modelling
124 studies that use steady-state circulation models. Among other advantages over existing so-
125 lutions (i.e., the AO), AIBECS.jl offers better computational efficiency, enhanced versatility,
126 composability with other Julia packages, and ease of reproducibility (granted by version con-
127 trol and Julia's package manager) and improved syntax, which are pillars of modern scientific
128 dissemination. Thus, AIBECS users may include sea-going oceanographers and educators who
129 will benefit from its simplicity, as well as more experienced modellers who can leverage its
130 computational advantages. AIBECS.jl has been used for teaching and is currently used for
131 research focused on marine trace metals.

132 The publication of circulation models as transport matrices from existing general circula-
133 tion models (Bardin et al., 2014, 2016; Khatiwala et al., 2005; Khatiwala, 2007; Kvale et al.,
134 2017; Zanna et al., 2019), and hopefully, future publication of transport matrix estimates from
135 standard ocean general circulation models (e.g., Chamberlain et al., 2019) will increase the
136 collection of circulations available from AIBECS.jl. Of particular interest to the broader com-
137 munity to facilitate the simulation of past and future marine biogeochemical states would be
138 transport matrix models extracted from the Climate Model Intercomparison Project (CMIP),
139 which includes past and future simulations of the ocean circulation.

140 Further devepment could include exposing advanced Grren-function-based diagnostic tools
141 (e.g., Holzer et al., 2021; Pasquier & Holzer, 2018), coupling tracers on different grids,
142 Newton–Krylov solvers for cyclo-stationary states (e.g., CYCLOCIM: Huang et al., 2021), or
143 time-dependent solvers for transient biogeochemical simualtions provided, e.g., by the SciML

144 ecosystem (Rackauckas & Nie, 2017). Bridging packages could be implemented for improved
145 composability with statistical packages (e.g., Turing.jl: Ge et al., 2018), optimization tools,
146 and plotting software (e.g., Makie.jl: Danisch et al., 2021; Danisch & Krumbiegel, 2021).

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