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Open-source stand-alone version of atmospheric model Aeolus 2.0 software

Masoud Rostami^{1,2} | Stefan Petri¹ | Sullyandro Oliveira Guimarães¹ | Bijan Fallah¹

¹Potsdam Institute for Climate Impact Research (PIK), Leibniz Association, Potsdam, Germany

²Laboratoire de Météorologie Dynamique (LMD), Sorbonne University (SU), Ecole Normale Supérieure (ENS), Paris, France

Correspondence

Masoud Rostami, Potsdam Institute for Climate, Impact Research (PIK), Leibniz Association, P.O. Box 60 12 03, Potsdam D-14412, Germany.
Email: rostami@pik-potsdam.de and masoud.rostami@lmd.ipsl.fr

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Abstract

In this discourse, we present the unveiling of an open-source software package designed to facilitate engagement with the atmospheric model, Aeolus 2.0. This particular iteration stands as a self-contained model of intermediate complexity. The model's dynamical core is underpinned by a multi-layer pseudo-spectral moist-convective Thermal Rotating Shallow Water (mcTRSW) model. The pseudo-spectral problem-solving tasks are handled by the Dedalus algorithm, acknowledged for its spin-weighted spherical harmonics. The model captures the temporal and spatial evolution of vertically integrated potential temperature, thickness, water vapour, precipitation, and the intricate influence of bottom topography. It comprehensively characterizes velocity fields in both the lower and upper troposphere, employing resolutions spanning a spectrum from the smooth to the coarse, enabling the exploration of a wide range of dynamic phenomena with varying levels of detail and precision.

KEYWORDS

Aeolus 2.0, atmosphere model, moist-convection, open source, thermal rotating shallow water model

1 | INTRODUCTION

A growing disparity between the intricate global climate model simulations and simplified theoretical approaches poses a challenge for climate scientists to gain a comprehensive understanding of the underlying physical mechanisms and phenomena. Bridging this gap demands a hierarchical approach to research, as advocated by Held (2005). The proliferation of parameterizations for physical processes in General Circulation Models (GCMs) often obscures the individual significance of each process, such

as the water vapour cycle, moist convection, and radiative transfer, within the synoptic-scale atmospheric dynamics. Failing to establish appropriate model hierarchies may result in models becoming “black boxes,” hindering our capacity to enhance them further. To address this challenge, a series of hierarchical models becomes indispensable. Among these, we present our in-house model, Aeolus 2.0.

The widely employed Rotating Shallow Water (RSW) model has proven valuable for investigating atmospheric and oceanic flows. It integrates the atmospheric primitive equations using pseudo-height isobaric vertical

Dataset information available in the link <https://zenodo.org/records/10823194>.

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coordinates, enabling the capture of critical features of large-scale fluid dynamics, including jet streams and Rossby waves (Zeitlin, 2018). However, the classical RSW model has limitations, notably in its neglect of horizontal gradients of potential temperature and the influence of moist convection, both of which are significant in specific atmospheric and oceanic contexts. These effects, driven by the interaction between temperature and water vapour content, lead to the formation of clouds, precipitation, and other atmospheric features. To overcome these limitations, researchers have developed modified RSW models, such as the moist-convective Thermal Rotating Shallow Water (mcTRSW) model (Rostami & Zeitlin, 2022). The mcTRSW model incorporates horizontal gradients of potential temperature and moist convection, enhancing the accuracy of atmospheric current simulations beyond that of classical RSW models. This, in turn, makes the mcTRSW model an ideal choice for the investigation of fully nonlinear adjustments of large-scale positive buoyancy anomalies in a moist-convective setting (Rostami et al., 2024) and extreme events. It offers valuable insights into the intricate interplay between temperature, water vapour content, and large-scale atmospheric dynamics.

The model utilized in this study is supported by a theoretical foundation with a historical record for the incorporation of moist convection. The model is based on the moist-convective Rotating Shallow Water (mcRSW) model, which has already incorporated phase transitions of water vapour and the related latent heat release (Bouchut et al., 2009; Lambaerts et al., 2012; Lambaerts, Lapeyre, & Zeitlin, 2011; Lambaerts, Lapeyre, Zeitlin, & Bouchut, 2011). The evolution of the vertically averaged humidity and the corresponding effects of condensation and latent heat release on the air column are defined in the mcRSW model in a simple and consistent way, following the seminal ideas of Gill (1982). The mcRSW model has been continuously improved, and the applied version in this study includes additional features such as precipitable water, vapourization, and precipitation, as proposed by (Rostami & Zeitlin, 2018). This improved model has been used in numerous studies to investigate the effects of moist convection on the dynamics of large-scale Earth and planetary jets and vortices (Lahaye & Zeitlin, 2016; Lambaerts et al., 2012; Rostami et al., 2017; Rostami & Zeitlin, 2017, 2019a, 2019b, 2020b, 2022).

The dynamical core of Aeolus 2.0 is a multi-layer mcTRSW model. The theoretical foundation of the multi-layer TRSW model, applicable to both diabatic “dry” and moist-convective conditions, is expounded in Rostami et al. (2022), where it distinguishes itself with its remarkable ability to capture the dynamics of extreme weather phenomena like the Madden-Julian Oscillation (MJO). In contrast to traditional shallow-water models, which

assume homogeneity, incompressibility, and hydrostatic balance, TRSW models incorporate inhomogeneous layers, allowing for horizontal variations in material properties. The model is constructed upon the vertical integration of atmospheric primitive equations using pseudo-height isobaric vertical coordinates (see Figure 1). It accurately represents horizontal gradients of potential temperature and their evolution due to moist convection, providing an internally consistent and transparent approach. The mcTRSW model excels by fully embracing the nonlinearity inherent to moist convection, incorporating factors such as latent heat release, the phase transition of moist air, and the evolving buoyancy field. This empowers the model to dissect intricate aspects of extreme weather events, encompassing heat fluxes and the pivotal role of moist convection. Aeolus 2.0 takes into account bottom topography, while incorporating insolation, short-wave, and long-wave radiation effects through the rapid radiative transfer (RRTM) model (Mlawer et al., 1997). It also considers precipitable water and the vapourization of condensed water, elevating its capability to perform atmospheric simulations with intermediate complexity. We parameterize Cloud Liquid Water Content (CLWC) using the Betts-Miller method (Betts & Miller, 1986). The numerical methods used in Aeolus 2.0 are based on the Dedalus project (Lecoanet et al., 2019; Vasil et al., 2019). Dedalus solves differential equations using spin-weighted spectral methods. Dedalus is a Python 3 package (<https://dedalus-project.org/>) comprising custom C-extensions (compiled with Cython) and dependent on several essential scientific libraries and tools, including MPI (Message Passing Interface), FFTW (Fastest Fourier Transform in the West), HDF5 (Hierarchical Data Format version 5), and a fundamental scientific Python stack that encompasses numpy, scipy, mpi4py, and h5py. This framework equips Dedalus with the capabilities needed for efficient and high-performance scientific computations.

The various levels of complexity that can be configured in the model include the following:

- The desired structure can be simulated in a diabatic “dry” environment both with and without bottom topography.
- The desired structure can also be simulated in an adiabatic moist-convective environment, again both with and without bottom topography.
- In addition, the desired structure can be simulated in an adiabatic moist-convective environment with bottom topography, insolation, seasonal variation, and Rapid Radiative Transfer Model (RRTM; (Mlawer et al., 1997)), which captures the effects of greenhouse gases and common halocarbons. The model is based on a combination of line-by-line and correlated-k

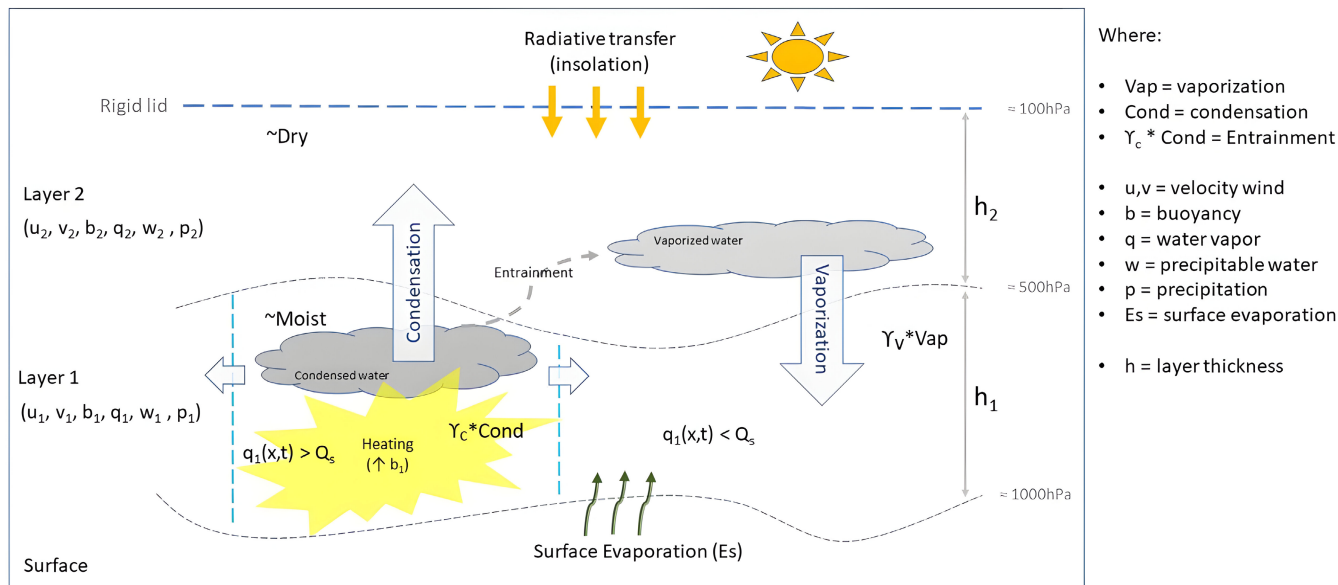


FIGURE 1 Illustration of a schematic depicting the conceptual framework of a two-layer moist-convective Thermal Rotating Shallow Water (mcTRSW) model, showcasing its fundamental structure and key components for atmospheric simulations.

approaches, which allows it to accurately calculate the radiative transfer properties of both highly and weakly absorbing gases. The vertical structure of the RRTM is based on a series of discrete vertical layers that are defined by the user.

2 | REQUIRED LIBRARIES AND PACKAGES FOR THE MODEL

The model relies on several essential libraries and packages. Below is a comprehensive list of these requisite resources:

- `sys`: The ‘`sys`’ module furnishes functions and variables for seamless interaction with the Python interpreter.
- `os`: The ‘`os`’ module offers cross-platform functionality for accessing and utilizing operating system-dependent features.
- `time`: The ‘`time`’ module boasts a variety of time-related functions, including the precise measurement of elapsed time.
- `json`: The ‘`json`’ module facilitates the manipulation and processing of JSON (JavaScript Object Notation) data.
- `argparse`: The ‘`argparse`’ module presents a versatile mechanism for parsing and handling command-line arguments, enhancing the model’s configurability.
- `xarray`: ‘`xarray`’ is a powerful library tailored for the manipulation of labelled multi-dimensional arrays, which is integral to data handling in the model.
- `numpy`: ‘`NumPy`’ stands as a foundational package, indispensable for scientific computation within the Python ecosystem, supporting the model’s numerical operations.
- `scipy.integrate`: The ‘`scipy.integrate`’ module endows the model with sophisticated tools for the integration of Ordinary Differential Equations (ODEs), enabling the modelling of dynamic processes.
- `scipy.special`: The ‘`scipy.special`’ module provides an extensive collection of specialized functions, enriching the model’s capabilities for advanced mathematical operations.
- `scipy.io`: The ‘`scipy.io`’ module equips the model with the means to efficiently handle various file formats, a vital component for data exchange and storage.
- `mpi4py`: The ‘`mpi4py`’ library supplies Python bindings for the Message Passing Interface (MPI), an imperative element for high-performance parallel computing.
- `dedalus.public`: The ‘`dedalus.public`’ module is a fundamental component of the Dedalus framework, purpose-built for solving partial differential equations (PDEs). The corresponding libraries and modules within Dedalus are indispensable for the model’s execution.
- `timesteppers`: This bespoke module, adapted from Dedalus, is intrinsically connected to time-stepping methods, optimizing temporal integration in the model.
- `NetCDFOutput`: ‘`NetCDFOutput`’ is a custom module tailored for streamlined interaction with NetCDF (Network Common Data Form) files, a prevalent format for storing multi-dimensional scientific data.

- climlab: ‘climlab’ is a comprehensive library specifically designed for process-oriented climate modelling, offering advanced tools for investigating various atmospheric and environmental phenomena. Furthermore, specific submodules from ‘climlab’ including ‘constants’, ‘daily_insolation’, ‘orbitalTable’, and ‘pseudoadiabat’ are indispensable to the model, enriching its capacity for simulating complex climate interactions.
- jacob128.py, sphere128.py, sphere_wrapper.py: These scripts, adapted from Dedalus, convert spin-weighted spherical harmonic parameters into Jacobi parameters or other necessary parameters.

3 | PSEUDO-SPECTRAL NUMERICAL METHOD AND SETUP

In this section, we will refrain from reiterating the fundamental dynamics and theoretical underpinnings of Aeolus, 2.0, as comprehensively detailed in prior works such as Rostami et al. (2022) and Rostami et al. (2024). However, we will outline several pivotal features that characterize the model. Aeolus, 2.0 harnesses the power of parallel computing, enabling the distribution of computational tasks for faster and more efficient simulations. The file README.txt contains the installation and running instructions for the model. Numerical methods employed in the model are based on the Dedalus algorithm, which utilizes spin-weighted spherical harmonics (Lecoanet et al., 2019; Vasil et al., 2019). Spin-weighted spherical harmonics were first introduced by Gelfand and Shapiro (1956) in their Lorenz group studies. One significant advantage of spin-weighted spherical harmonics is that when combined with spinor basis vectors, they simplify differentiation on the sphere, making it similar to Fourier series, where diagonal wavenumber multiplication remains regular everywhere. This eliminates the need for handling traditional singular gradients at the poles. The spectral discretizations utilize the Fourier spectral basis for each spatial dimension. It is worth noting that other methods have been proposed to address coordinate singularities in spheres and disks (Boyd & Yu, 2011). The schematic representation of a spin-weighted spherical harmonic transform for a set of shallow water equations is as follows:

$$\partial_t u + g \nabla h + 2\Omega e_z \times u = F - u \cdot \nabla u, \quad (1a)$$

$$\partial_t h + H \nabla \cdot u = F(h) - \nabla \cdot (hu), \quad (1b)$$

Here, u is a 2D velocity field in spherical coordinates, represented as $u = u_\phi e_\phi + u_\theta e_\theta$. The unit vectors on the surface

of the sphere are e_θ and e_ϕ , with $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$, representing polar and azimuthal angles, respectively. Velocity field and unit vectors on a spin-weighted basis are defined as follows:

$$u_\pm = \frac{1}{\sqrt{2}}(u_\theta \pm iu_\phi), \quad e_\pm = \frac{1}{\sqrt{2}}(e_\theta \mp ie_\phi). \quad (2)$$

The transformed equations from (1) become

$$\partial_t u_+ + g \nabla_+ h + i2\Omega \cos(\theta) u_+ = F_+ - [u \cdot \nabla u]_+, \quad (3a)$$

$$\partial_t u_- + g \nabla_- h - i2\Omega \cos(\theta) u_- = F_- - [u \cdot \nabla u]_-, \quad (3c)$$

$$\partial_t h + H(\nabla_+ u_- + \nabla_- u_+) = F(h) - \nabla_+(hu)_- - \nabla_-(hu)_+, \quad (3d)$$

where $\nabla_\pm = (1/\sqrt{2})(\nabla_\theta \pm i\nabla_\phi)$. For a comprehensive description of calculus for vector and tensor operations on the unit 2-sphere with spin-weighted spherical harmonics and a comparison with traditional methods, refer to Vasil et al. (2019). By specifying a dealiasing scale factor of 3/2, a global grid of 384 by 768 is set along the latitudinal and longitudinal directions, respectively. Additionally, two other grid resolutions are available for low-cost and fast simulations. The two-layer mcTRSW is calibrated with the barotropic equatorial Rossby deformation radius, $L_d = (\sqrt{gH}/\beta)^{1/2}$,

where $H = H_1 + H_2$, and H_1 and H_2 can be initialized according to the specific study. Here, β represents the gradient of the Coriolis force in the meridional direction. The zonal and meridional velocity, time, and Earth radius scales are as follows:

$$L \sim L_d, \quad (u, v) \sim \beta L_d^2, \quad t \sim \frac{1}{\beta L_d}, \quad a \sim L_d. \quad (4)$$

A value of $a/L_d = 1.7$ is chosen, but other ratios such as $a/L_d = 1.0, 1.5$, and 1.88 have been tested to assess the qualitative validity of the results.

Users have the flexibility to apply external forcing. For example, the initial non-dimensional thickness anomaly, as described by a simplified α -Gaussian equation, is provided in the model:

$$h' = h - H = \hat{h} \sqrt{2e} \frac{2^{1/\sigma}}{\sigma} \Gamma\left(\frac{1}{\sigma} + \frac{1}{2}\right) G\left(\frac{r^\sigma}{2}, \frac{1}{\sigma} + \frac{1}{2}\right), \quad (5)$$

Here, r represents the spherical distance, which is calculated using the function \mathcal{D} as follows: $r = \mathcal{D}(\text{Lat}_0, \text{Lon}_0, \text{Lat}, \text{Lon}) = \mathcal{D}(0, 0, \lambda/r_{as}, \Phi)/L_h$. In this context, r_{as} determines the aspect ratio, while L_h influences the spatial perturbation sizes. It is important to note that the specific values chosen for L_h , r_{as} , and σ can

be arbitrary and adjusted based on the requirements of the study. The calculation of r is based on the great-circle distance with respect to the reference point using the Haversine formula. $\Gamma(x)$ denotes the Gamma function, and $G(r, a)$ is the incomplete Gamma function. The parameters \hat{h} and σ determine the amplitude and steepness of the thickness anomaly, respectively. The water vapour in the conceptual configuration is initialized uniformly and close to the saturation value, denoted as Q^s . In contrast, the upper layer is initialized far from the saturation value. The initial conditions can be adjusted to meet the specific requirements of the study. In a realistic configuration with actual topography, the model needs to be initialized with data corresponding to the desired year. In particular, non-dimensional velocity and buoyancy fields are crucial for running the model effectively. If there are no initial conditions for water vapour in a realistic configuration, the model will reach an equilibrium state within just a few days due to forced surface evaporation. Figure 2 portrays a representative data output, illustrating the interplay of precipitation and buoyancy fields, which have been averaged on a monthly basis for the specific temporal window of January 1980. These fields are derived as a result of input data originating from the ERA5 dataset. It is worth noting that the parameters of surface evaporation in this published version of Aeolus 2.0 have not been well calibrated with respect to observational data. Further investigation is pending, and the results will be published in the upcoming months.

The model offers an additional optional feature, allowing it to be initialized in a nonlinear, adjusted thermo-quasi-geostrophic balanced state. This initialization is carried out by providing the necessary buoyancy and velocity fields.

The model produces more accurate and converged solutions by employing higher resolutions. It has been tested for the benchmark problem of Gill's mechanism, as presented in Rostami et al. (2022). This benchmark

involves the propagation of eastward fronts of buoyancy and condensation fields due to a significant buoyancy anomaly in the lower layer. The model successfully captures (sub)mesoscale instabilities arising from thermal effects and the nonlinearity of moist convection during these extreme events. The results are consistent with those of the RSW model with a finite volume scheme (cf. Rostami & Zeitlin, 2020a).

The TRSW dynamical core exhibits a distinctive trait as a layer model, diverging significantly from conventional level models prevalent in geophysical fluid dynamics. In the realm of atmospheric and oceanic representation, layer models and level models offer contrasting methodologies for delineating the vertical structure. While level models seamlessly incorporate thermodynamic considerations, their effectiveness diminishes notably, especially in scenarios requiring high vertical resolutions. The fundamental difference between layer and level models lies in their treatment of density profiles. Level models typically assume a continuously stratified density, employing finite differencing techniques at fixed depths. Conversely, layer models adopt an approximation strategy, discretizing the density profile into piece-wise constant segments, where the interfaces' depth can dynamically evolve with spatial and temporal dynamics. The inherent accuracy challenges in level models stem from finite differencing constraints, particularly notable at smaller spatial scales. In contrast, layer models circumvent such limitations by adopting a piece-wise constant density profile, a physically plausible representation where the equations of motion faithfully capture this stratified structure.

Highlighting this difference, the Laplace tidal equations provide a clear example of how layer and level models diverge. These equations, essential for explaining tidal behaviour in both the ocean and the atmosphere, embody a one-layer model approach that is noticeably absent in level modelling frameworks.

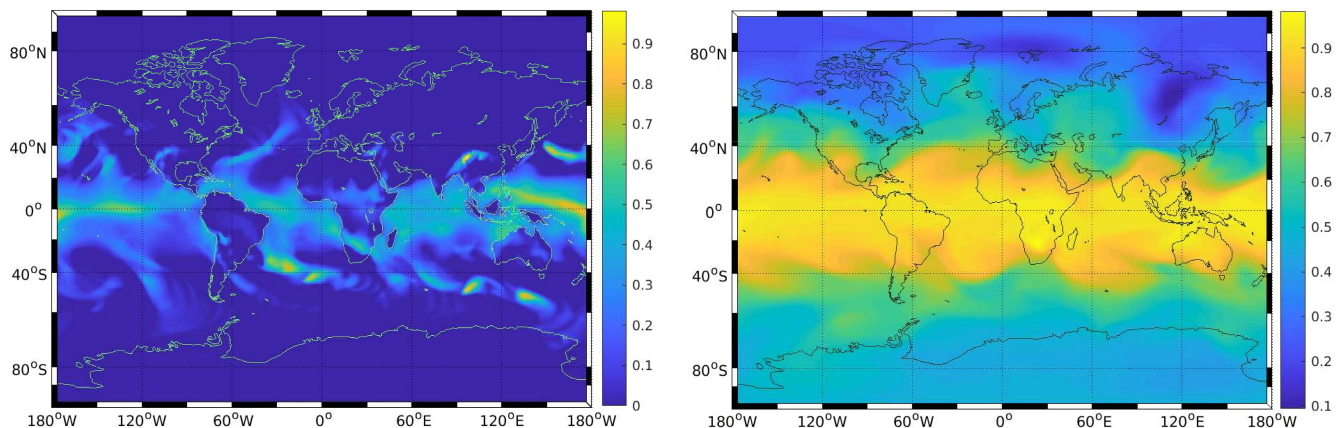


FIGURE 2 Monthly normalized precipitation (left panel) and buoyancy (right panel) fields simulated by Aeolus 2.0 for January 1980, utilizing input data from ERA5.

4 | FUTURE DEVELOPMENTS

The practical implementation of multi-layer Thermal Rotating Shallow Water (TRSW) models on a spherical domain within atmospheric models has been a rare and under-explored endeavour. To the best of our current knowledge, Aeolus 2.0 stands as a pioneering open-source atmospheric model in this category, aiming to incorporate a wide range of non-adiabatic effects. It is important to acknowledge that, at this stage, the model is in its nascent phase.

Anticipated future developments for Aeolus 2.0 encompass a range of enhancements. A primary focus will be the refinement of the moist-convective scheme, designed to accurately represent the complexities of both sea and land surface evaporation. This is crucial for achieving a higher degree of realism in simulating real-world atmospheric conditions. Furthermore, there is a commitment to improving parametrization, with the aim of establishing an energy balance and Hamiltonian structure, especially during transitions to moist-convective and radiative transfer regimes.

Aeolus 2.0 exhibits the potential in simulating various phenomena crucial to climate dynamics, including the poleward expansion of warm zones, assessing the effects of global warming on atmospheric structures like synoptic-scale mid-latitude jets and cyclones, understanding energy transfer mechanisms from tropical regions to mid-latitudes, examining global precipitation patterns under changing climate conditions, and modelling extreme events, such as heat waves, Madden-Julian Oscillation (MJO), and El Niño-Southern Oscillation (ENSO).

User feedback and ongoing research on extreme events will serve as valuable resources for refining and advancing the model. The scientific community's input, experiences, and insights will play an instrumental role in Aeolus 2.0's continuous improvement.

A visionary step in Aeolus 2.0's evolution involves its integration with the Potsdam Earth System Model (POEM) as one of its atmospheric components. This marks a significant progression towards a comprehensive Earth system modelling framework that encapsulates the intricate interactions and feedback mechanisms between the atmosphere, oceans, land surface, and biosphere. Such a coupling would facilitate holistic investigations into the complex dynamics of the Earth's climate system.

5 | CONCLUSIONS

In this discourse, we introduce Aeolus 2.0, an open-source software package tailored to facilitate engagement with

the atmospheric model of intermediate complexity. This model incorporates a multi-layer pseudo-spectral moist-convective Thermal Rotating Shallow Water (mcTRSW) framework, effectively capturing the temporal and spatial evolution of critical atmospheric variables.

Aeolus 2.0 bridges the gap between complex global climate models and simplified theoretical approaches, offering a hierarchical solution to study the intricate dynamics of atmospheric processes. It extends beyond the conventional Rotating Shallow Water (RSW) model by accounting for horizontal gradients of potential temperature and the influence of moist convection. This modification significantly enhances the accuracy of atmospheric current simulations, making it well-suited for investigating large-scale positive buoyancy anomalies, moist-convective settings, and extreme weather events.

The model's dynamical core is founded on the principles of multi-layer TRSW, making it adaptable to various environmental scenarios. It departs from traditional shallow-water models by embracing the nonlinearity inherent to moist convection. The incorporation of factors like latent heat release and phase transitions of moist air allows Aeolus 2.0 to dissect intricate aspects of extreme weather events, including heat fluxes and the pivotal role of moist convection. The model is also equipped to consider bottom topography, insolation, radiation effects, and precipitable water, further enhancing its ability to simulate complex atmospheric interactions.

The numerical methods employed in Aeolus 2.0 are based on the Dedalus algorithm, utilizing spin-weighted spherical harmonics. This approach simplifies differentiation on the sphere and eliminates singular gradients at the poles, making it ideal for global atmospheric simulations. By offering different grid resolutions, the model provides flexibility for low-cost and fast simulations.

Aeolus 2.0 also allows for external forcing and offers an optional initialization feature with nonlinear adjusted thermo-quasi-geostrophic balanced states, incorporating necessary buoyancy and velocity fields.

In summary, Aeolus 2.0 represents a tool for atmospheric scientists and researchers seeking to explore a wide range of dynamic phenomena with varying levels of detail and precision. Its hierarchical approach and advanced modelling capabilities make it a significant contribution to the field of atmospheric science, facilitating more comprehensive insights into complex atmospheric processes.

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CONFLICT OF INTEREST STATEMENT

The authors report no conflict of interest.

OPEN RESEARCH BADGES



This article has been awarded Open Data Badge for making publicly available the digitally-shareable data necessary to reproduce the reported results. Data is available at <https://zenodo.org/records/10823194>.

DATA AVAILABILITY STATEMENT

Aeolus 2.0 has been uploaded to Zenodo and is available via the following link: [10.5281/zenodo.10054154](https://zenodo.org/records/10054154). Please note that the last updated version of the model will also be accessible through the same link. We would like to highlight that the software utilized in this study is licensed under the Creative Commons Attribution 4.0 International Licence, granting users the freedom to use and adapt the code for their research needs.

ORCID

Masoud Rostami <https://orcid.org/0000-0003-1730-5145>

Stefan Petri <https://orcid.org/0000-0002-4379-4643>

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