An Emulator-Based Modelling Framework for Studying Astronomical Controls on Ocean Anoxia with an Application on the Devonian

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Abstract. We present a modelling framework to study the response of continental flux dynamics and ocean anoxia to astronomical forcing. The GEOCLIM model is coupled with a Gaussian Process-based climate emulator, designed to efficiently capture the global distribution of temperature and precipitation as simulated by the general circulation model HadCM3. The emulator employs principal component analysis for dimensionality reduction. Compared to earlier approaches, our emulator features an additive kernel function that better captures the spatial complexity of ocean responses and accounts for ocean heat transport. This setup facilitates interactive coupling between CO_2 levels through an iterative procedure involving GEOCLIM and the emulator, enabling systematic exploration of various orbital and pCO_2 configurations. We demonstrate the model's capabilities with an application aimed at investigating plausible mechanisms behind Devonian anoxia.

1 Introduction

Modelling long-term climate dynamics and related environmental phenomena presents significant challenges, particularly when investigating events from deep geological time. These challenges can stem from various uncertainties in boundary conditions, forcing mechanisms, and geological reconstructions, which significantly complicate model parameters tuning, or in the timescales involved. This paper presents a modelling framework specifically designed to investigate the connection between astronomical forcing, biogenic fluxes, and anoxia, with an application to the Devonian period (419 to 359 million years ago). The Devonian serves as an excellent test case, as it was characterized by significant climatic and environmental transformations, including 29 instances of ocean anoxic or hypoxic conditions (Becker et al., 2020).

The dynamics of these Ocean Anoxic Events (OAEs), and the responsible mechanisms, have been investigated over the last decades, but failed to yield consensus (see for instance Haddad et al. (2018)). It has been hypothesized that the cyclical recurrence of anoxia in geological records can be influenced by astronomical cycles within a broader context of background environmental conditions (c.f., De Vleeschouwer et al., 2017; Whalen et al., 2017; Da Silva et al., 2020; Lu et al., 2021; Ma

et al., 2022, 2025; Wichern et al., 2024). These cycles involve changes in the rotation of the Earth's axis and the geometry of its orbit, which impact seasonal variations and the level of incoming solar radiation, thereby affecting the global climate (see Berger and Yin (2021) or Zeebe and Kocken (2024) for an introduction on astronomical forcing.). Specific configurations of the astronomical forcing would help triggering regional or even possibly global anoxia in a context of already low-oxygen con-
25 tent. Furthermore, orbital forcing would pace anoxia bursts. One suggested mechanism involves the influence of astronomical forcing on the position of tropical precipitation. Such changes would affect the dynamics of nutrient storage on the continent, as well as the rate and time at which they are released in the oceans. Finally, the modulation of nutrient release would impact ocean biogeochemistry (De Vleeschouwer et al., 2017, 2024; Wichern et al., 2024).

In the specific case of the Devonian, De Vleeschouwer et al. (2017) and Wichern et al. (2024) suggest that conditions for
30 triggering and sustaining anoxia may best be met after passage through a so-called node of the very-long eccentricity cycle: a configuration met approximately every 2.4 million years (Laskar, 2020). However, as the precise timing of astronomical forcing during the Paleozoic is uncertain due to the chaotic nature of planetary dynamics, the investigation strategy needs to consider different scenarios. Furthermore, the anoxia itself may have a duration ranging from several tens of thousands to approximately one hundred thousand years, which poses additional questions about sustaining mechanisms. A possible explanation would be a
35 positive feedback loop involving nutrient recycling (Reershemius and Planavsky, 2021; De Vleeschouwer et al., 2024; Wichern et al., 2024).

To properly investigate the relationship between astronomical forcing and biogenic fluxes leading to anoxia, we need modelling tools capable of spanning geological timescales. The GEOCLIM framework (Donnadieu et al., 2006; Arndt et al., 2011; Goddéris and Donnadieu, 2019; Maffre et al., 2021) has been developed as a versatile suite of models designed to dynamically
40 simulate geochemical cycles and regolith (i.e., the upper layer of the continental crust where chemical weathering occurs) dynamics over long timeframes. However, realistically estimating the response of atmospheric conditions, particularly the impact of astronomical forcing on rainfall patterns that control nutrient mobilization, is challenging. While General Circulation Models (GCMs) produce adequate representations of ocean and atmosphere dynamics, integrating such models over the millions of years necessary to probe the dynamics of accumulation and release of nutrients for multiple astronomical scenarios is
45 impractical.

In light of these challenges, a solution is to develop a climate emulator calibrated on a plan of experiments with a GCM. This emulator-based approach allows us to capture the spatial complexity of the ocean-atmosphere response to astronomical forcing as simulated by the GCM, while requiring minimal computational resources once trained. This efficiency enables the systematic exploration of multiple astronomical scenarios and their impact on nutrient fluxes and ocean anoxia, making it a
50 practical tool for investigating the hypothesized connection between astronomical forcing and Devonian OAEs.

In this work, we have developed and tested an emulator, and the objective of this paper is to provide a comprehensive description of it, along with the justification for our technical choices. This will serve as a robust reference for further analysis of the climatic mechanisms governing astronomical control over biogenic fluxes and anoxia.

More precisely, we consider the framework proposed by Bounceur et al. (2015); Lord et al. (2017); Van Breedam et al.
55 (2021) of constructing the structure of the emulator based on the theory of Gaussian Processes (GPs, MacKay et al., 1998;

Rasmussen, 2006). This study advances the GEOCLIM framework by introducing a dynamically coupled emulator that enables bidirectional interaction. The geochemical model determines CO_2 levels, which the emulator then translates into climate predictions affecting continental weathering and erosion, and consequently nutrient fluxes. These, in turn, influence subsequent geochemical calculations, allowing for an iterative feedback process that can reveal how astronomical forcing ultimately

60 impacts continental fluxes and ocean biogeochemistry. It is essential to ensure that the GP emulator is robust enough for integration into a coupled soil-biogeochemical model. Though we illustrate its use on the Devonian, the methodology remains applicable to other geological periods. Additionally, compared to earlier work, we aim to account for changes in surface ocean dynamics and the related ocean heat transport caused by the astronomical forcing.

2 Methods

65 Following the definition by Kennedy and O'Hagan (2000); Oakley and O'Hagan (2002); Wilkinson (2010), an emulator is a statistical model that predicts the output of climate conditions provided by a 'simulator', here a GCM, in response to input parameters. The emulator must first be trained with a set of experiments with the GCM; the experiment set is designed such as to efficiently probe an input parameter space. Once trained, the emulator enables swift approximations of climate outputs, thereby allowing us to explore scenarios that would be practically impossible to produce through a traditional GCM usage.

70 To construct the climate database used to train the emulator, we decided to employ two types of GCMs: a coupled ocean-atmosphere model and a lighter, computationally less expensive model where the ocean is represented by a flat layer called a slab (we hereafter call it the slab model). We follow a two-tier approach by which we calibrate the slab model with the coupled one, and then produce a larger set of experiments with the slab model to generate the data needed to train the emulator. This double-layer strategy enables us to capture essential atmospheric dynamics accounting for changes in ocean heat transport

75 while mitigating the computational cost. We now give the technical details of this procedure.

2.1 Geophysical models setup and boundary conditions

2.1.1 HadCM3L and HadSM3

The Hadley Centre Coupled Model version 3 Low Resolution (HadCM3L) serves as our primary reference GCM for simulating Devonian climate conditions. The spatial resolution of $3.75°$ longitude $\times$ $2.5°$ latitude for both the atmosphere and oceanic

80 grid can adequately capture the essential mechanics of monsoonal systems. Albedo, snow accumulation, vegetation and soil processes were computed using the MOSES-II land-surface scheme (Cox et al., 1999, 2000; Cox, 2001; Essery et al., 2001). For a comprehensive description of the model's technical aspects, the reader is directed to its descriptive paper (Valdes et al., 2017).

HadSM3 is the slab version of HadCM3 where the atmosphere is coupled to a simple non-dynamic mixed layer ocean

85 (Williams et al., 2005). This simpler model is computationally efficient in two ways: ocean dynamics are by-passed, and a
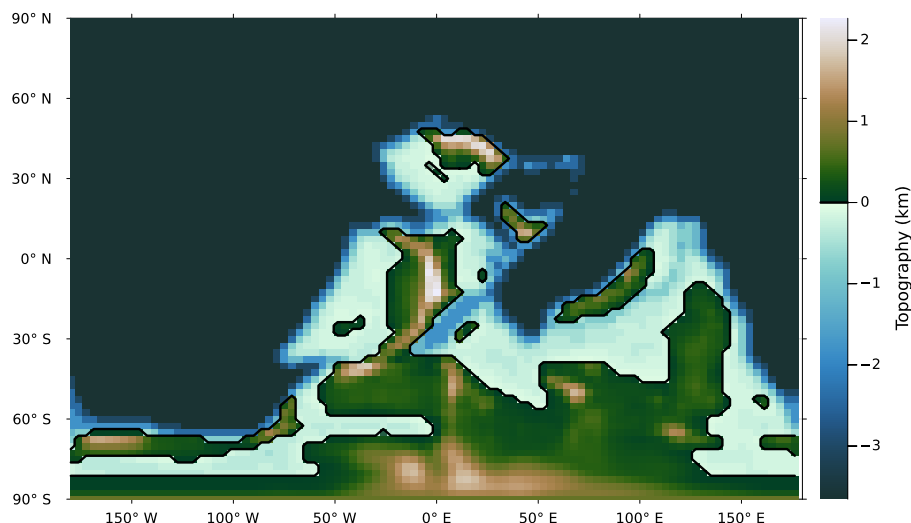
Figure 1. Topography of the late Devonian (370 Ma) according to Scotese and Wright (2018) paleo-digital elevation model, and downscaled to match the grid resolution of HadCM3L.

stationary solution can be found after an integration of ca. 30 years, compared to 5000+ years with HadCM3 (Valdes et al., 2021). Hence, it will be used here to perform a larger number of experiments.

The model uses large input files called *dumps*, which contain initial and boundary conditions. Those used here are adapted from Valdes et al. (2021). The 370-Ma palaeogeography is obtained from the dataset of Scotese and Wright (2018), as depicted

90 in Figure 1. It was chosen with the intention to best represent the Earth's geometry during the Frasnian-Famennian boundary, coinciding with an OAE that triggered a mass extinction around 372 million years ago (Percival et al., 2018; Carmichael et al., 2019).

Given the slab ocean model's deficiency in ocean dynamics, the computation of a corrective flux, known as the anomalous heat convergence, is required to accurately represent sea surface temperatures (SSTs) and sea-ice concentration. This flux

95 represents the imbalance between the incoming and outgoing energy fluxes within the model and is used as a monthly forcing to best represent the first order atmosphere-ocean interaction.

To transition from the coupled model (HadCM3L) to the slab model (HadSM3), we follow a two-step approach. First, a series of 15 experiments were conducted using the coupled version of the model with varying orbital parameters. These experiments were run for 250 years, sufficient to achieve a near-equilibrium state in the upper ocean. For each experiment, the resulting

100 SST and sea-ice concentration fields from HadCM3L were then prescribed to the slab model to diagnose the Anomalous Heat Convergence. This heat convergence field represents the heat transport that would have been provided by ocean dynamics in the coupled model, allowing the slab model to replicate similar climate patterns despite its simplified ocean representation. Second, we use an Inverse Distance Weighting interpolation (IDW) to obtain appropriate heat convergence fields for our full

set of 81 experiments with different orbital configurations. Detailed information on this process and the explored parameter

105   space can be found in appendix A.

In every simulation, the palaeogeography and the solar constant (1322 Wm^{-2}, Bahcall et al., 2001) are set identical. The orbital parameters (eccentricity, longitude of the perihelion, and obliquity), the atmospheric CO_2 concentration and the monthly heat correction flux are constant in time, but are prescribed to different values for each experiment. Once these boundary conditions and parameters are established, HadSM3 is run for 80 model years, with the last 30 years averaged to

110   minimize interannual variability and accurately represent the annual climatic averages of key variables, such as temperature, evaporation, and precipitation.

2.1.2 GEOCLIM

GEOCLIM (Donnadieu et al., 2006; Arndt et al., 2011; Goddéris and Donnadieu, 2019; Maffre et al., 2021) is a versatile suite of models designed to dynamically simulate geochemical cycles over geological timescales. The core of the model structure is

115   COMBINE, an ocean-atmosphere chemistry model based on advection-reaction principles, using a discretization into 10 boxes representing nine oceanic and one atmospheric compartments. More precisely, we use version 6.1.0, which differs slightly from its newest version GEOCLIM7 (Maffre et al., 2024). However, the continental modules of both versions are the same, which is the key point of this study.

This model is integrated with an early diagenesis module responsible for calculating output fluxes, such as the burial of

120   elements in marine sediments across each box. Additionally, GEOCLIM features a continental module, which computes input fluxes and is spatially resolved using a geographic mesh grid. The resolution of this module is adaptable and includes a soil model based on previous work by Gabet and Mudd (2009) and West (2012).

GEOCLIM computes various geochemical cycles, including those of carbon, oxygen, alkalinity, phosphorus, and sulphur, within each reservoir. It dynamically simulates these cycles without assuming steady-state conditions, incorporating rapid

125   processes like ocean mixing and water column sedimentation under parametrized forms. However, it necessitates inputs from a climate model.

Within the continental module of GEOCLIM, Dynsoil accounts for physical erosion and silicate weathering. The other fluxes computed by the continental module are carbonate weathering, petrogenic organic carbon, phosphorus weathering, and terrestrial organic carbon export. Surface bedrock is categorized into lithological classes, and erosion and weathering processes

130   are solved dynamically over geological timescales. A more complete description of the model and its parametrizations can be found in the supplementary material of Maffre et al. (2021). A key aspect of Dynsoil is that it resolves the regolith thickness and computes the weathering fluxes accordingly. Here, we call *regolith* the interface between unweathered bedrock and the Earth's surface where chemical weathering reactions occur. It can be thought of as the layer of unconsolidated material that covers the bedrock. The regolith model describes a vertical profile of the abundance of primary minerals, beginning with an abundance

135   of 1 at the regolith/bedrock transition and decaying towards the surface as a result of dissolution. The Dynsoil module needs inputs of temperature and runoff (or precipitation and evaporation) over a spatial grid, which are typically supplied by a GCM or, here, the emulator of the GCM.

In summary, assuming adequate climate forcing, GEOCLIM's integration of continental processes, climate dynamics, and ocean biogeochemistry enables the comprehensive investigations of Earth system dynamics over multimillion-year timescales as needed for our general objective.

2.2 Experimental design

2.2.1 Parameter space

The inner solar system's dynamics exhibit chaotic behaviour, making it impossible to pinpoint an exact astronomical solution for the Late Devonian period. Only a handful of constraints on cycle frequencies, stabilities and amplitudes remain (Laskar et al., 2004, 2011b; Mogavero and Laskar, 2022; Zeebe and Kocken, 2024; Zeebe and Lantink, 2024).

Since the objective of this study is to construct climatologies for a plausible Late Devonian orbital configuration, it requires an extensive exploration of a broad domain. We focus on the response to four parameters: eccentricity e (which characterizes the shape of the Earth's orbit), longitude of the perihelion ϖ (the angular distance between the September equinox and the point in Earth's orbit where it is closest to the Sun – heliocentric convention), obliquity ε (the tilt of the ecliptic relative to the celestial equator), and the partial pressure of carbon dioxide in the atmosphere pCO_2.

The following intervals for each parameter were chosen to make sure that no extrapolation outside the domain will be needed:

$$e \in [0, 0.075] \tag{1}$$

$$\varpi \in [0, 2\pi[\tag{2}$$

$$\varepsilon \in [20.75°, 23.75°] \tag{3}$$

$$pCO_2 \in [1, 16] \times 280 \text{ ppm} \tag{4}$$

We propose the hypothesis that the prior basis $\{e\sin\varpi, e\cos\varpi, \varepsilon, \log_2(pCO_2)\}$, where $e\sin\varpi$ denotes the climatic precession and pCO_2 is expressed relative to pre-industrial levels (i.e., in units of 280 ppm), optimally encodes the initial distance metric among different climatologies. A more refined metric will be learned during the training phase of the GP emulator. This hypothesis is anchored in the interpretation of the climatic precession, where a large positive value signifies an excess of insolation in the Southern Hemisphere during the austral summer, and a large negative value indicates the same in the Northern Hemisphere during the boreal summer. Moreover, our prior judgement is that the globally averaged temperature responds by the same variation to every doubling of carbon dioxide concentration, hence the logarithm. Accordingly, we also define the rescaled CO_2 parameter:

$$m = \log_2\left(\frac{pCO_2}{280 \text{ ppm}}\right) \tag{5}$$

2.3 Construction and optimization of the training set

To construct the training set for the GP emulator, it is essential to sample the parameter space effectively to cover all regions of interest. For this reason, we use Latin Hypercube Sampling (LHS, Eglajs and Audze, 1977; Iman et al., 1981; McKay et al.,

2000). This method divides the range of each input parameter into equally probable intervals and selects one sample from each interval. Unlike direct random sampling, LHS provides a more uniform and comprehensive exploration of the parameter space, reducing redundancy and improving the representativeness of sampled points. This method is widely recognized for enhancing emulator accuracy and robustness (Urban and Fricker, 2010).

In this study, the LHS was further optimized using the Audze–Eglājs (AE) criterion (Eglajs and Audze, 1977; Eliáš and Vořechovský, 2016). The AE criterion was developed to optimize the spatial arrangement of points in a hypercube. This is achieved by expressing the potential energy of a system of particles where each pair of particles exerts a repulsive force on each other. These forces are functions of the distance between the pairs of points. By minimizing this potential energy, the AE criterion ensures a uniform and space-filling distribution of experimental points.

The optimization was executed in Julia, a high-level general-purpose dynamic programming language designed for high-performance numerical analysis and computational science (Bezanson et al., 2012), using a genetic algorithm (Bates et al.; Urquhart et al., 2020).

For our application, we must also account for some specificities of the input parameters. Indeed, uniformly sampling the climatic precession and coprecession would lead to unwanted high eccentricity experiments. This is resolved by making a change of variables and sampling uniformly $\{e^2, \varpi, \varepsilon, m\}$. Doing so also requires adapting the distance function in the optimization algorithm from Euclidean to

$$d_{ij} = \tilde{e}_i^2 + \tilde{e}_j^2 - 2\tilde{e}_i\tilde{e}_j\cos(\varpi_i - \varpi_j) + (\tilde{\varepsilon}_i - \tilde{\varepsilon}_j)^2 + (\tilde{m}_i - \tilde{m}_j)^2 \qquad (6)$$

where the tilde signifies that the value has been linearly rescaled to $[0, 1]$ interval for the eccentricity and $[-1, 1]$ for the obliquity and CO_2. This is necessary because the relative importances of eccentricity-modulated climate precession and obliquity for our variables of interest are a priori unknown. Ultimately, our input space will be optimally filled; climatic precession and coprecession will follow a semicircular distribution, while obliquity and m will be uniformly distributed.

In this work, based on the computational cost of HadSM3 and previous similar studies (Bounceur et al., 2015; Lord et al., 2017; Van Breedam et al., 2021), the number of samples has been arbitrarily fixed to 81.

3 Emulator development

The function of the emulator is to predict the output of HadSM3 for any input in the range spanned by the set produced with the procedure described in Section 2.3. Fundamentally, it is an interpolator: if it is well-designed and successfully validated, there is no need for further experiments using the GCM.

3.1 Theoretical basis of a Gaussian Process regression

We follow (MacKay et al., 1998; Rasmussen, 2006) Gaussian Processes (GPs), and specially, Gaussian Process Regression (GPR) to execute the interpolation procedure.
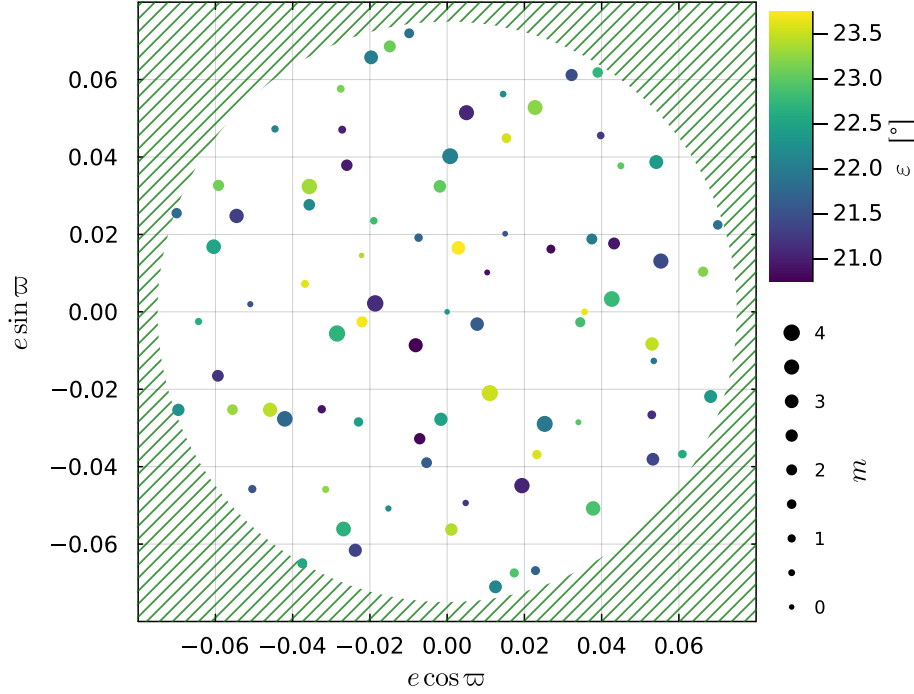
7

Figure 2. Projection of the experimental design onto the $\{e\sin\varpi, e\cos\varpi\}$ plane. Each point represent a GCM experiment. The color is associated to obliquity ε (in degree) and the marker size to carbon dioxyde $m = \log_2\left(\frac{p\mathrm{CO_2}}{280\,\mathrm{ppm}}\right)$. The dashed area is outside the range of the our maximal eccentricity $e_{\max} = 0.075$.

A GP (MacKay et al., 1998; Rasmussen, 2006) is a stochastic process, generally comprising random variables indexed by time or space. Its unique property is that any finite collection of these variables adheres to a multivariate Gaussian distribution. Therefore, a GP is a distribution over functions with a continuous domain, effectively describing a probability distribution over an infinite-dimensional vector space.

Let $\mathcal{Z} \subseteq \mathbb{R}^{n_z}$ be the index set, which is the number of input variables (in our case, $n_z = 4$). The function $f_{\mathrm{GP}}(\boldsymbol{z})$ with $\boldsymbol{z} \in \mathcal{Z}$ is a random variable. A GP is a stochastic process completely described by a mean function $m : \mathcal{Z} \to \mathbb{R}$ and a covariance function $k : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$ such that

$$f_{\mathrm{GP}}(\boldsymbol{z}) \sim \mathcal{GP}\left(m(\boldsymbol{z}), k(\boldsymbol{z}, \boldsymbol{z}')\right) \tag{7}$$

$$m(\boldsymbol{z}) = \mathbb{E}\left[f_{\mathrm{GP}}(\boldsymbol{z})\right] \tag{8}$$

$$k(\boldsymbol{z}, \boldsymbol{z}') = \mathbb{E}\left[\left(f_{\mathrm{GP}}(\boldsymbol{z}) - m(\boldsymbol{z})\right)\left(f_{\mathrm{GP}}(\boldsymbol{z}') - m(\boldsymbol{z}')\right)\right] \tag{9}$$

The covariance function serves as a measure of the correlation between two states $(\boldsymbol{z}, \boldsymbol{z}')$, and within the framework of GPs, is known as the kernel.

In Bayesian inference, the GP serves as the prior probability distribution, which can be used for function regression. This Bayesian approach merges new data with existing knowledge. Specifically, Bayes' theorem is employed to integrate the prior

with new data, resulting in a posterior distribution. The new data is represented as a training dataset $\mathcal{D} = \{\mathbf{X}, \mathbf{Y}\}$ where $\mathbf{X} = \left[\boldsymbol{x}_{\text{dat}}^{\{1\}}, \ldots, \boldsymbol{x}_{\text{dat}}^{\{n_{\mathcal{D}}\}} \right] \in \mathcal{Z}^{1 \times n_{\mathcal{D}}}$ (in our case $n_{\mathcal{D}} = 81$) is the input matrix and $\mathbf{Y} = \left[\tilde{y}_{\text{dat}}^{\{1\}}, \ldots, \tilde{y}_{\text{dat}}^{\{n_{\mathcal{D}}\}} \right]^{\top} \in \mathbb{R}^{n_{\mathcal{D}} \times 1}$ contains

215 the output values. The one-dimensional regression problem takes the following form

$$\tilde{y}_{\text{dat}}^{\{i\}} = f_{\text{GP}}(\boldsymbol{x}_{\text{dat}}^{\{i\}}) + \epsilon \tag{10}$$

for all $i \in \{1, \ldots, n_{\mathcal{D}}\}$ and $\epsilon \sim \mathcal{N}(0, \nu^2)$ is i.i.d. Gaussian measurement noise.

Considering that each finite subset of a GP follows a multivariate Gaussian distribution, we can construct the joint distribution for a random test point $\boldsymbol{z}^* \in \mathcal{Z}$:

$$
\begin{bmatrix} \mathbf{Y} \\ f_{\text{GP}}(\boldsymbol{z}^*) \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} m(\boldsymbol{x}_{\text{dat}}^{\{1\}}) \\ \vdots \\ m(\boldsymbol{x}_{\text{dat}}^{\{n_{\mathcal{D}}\}}) \\ m(\boldsymbol{z}^*) \end{bmatrix}, \begin{bmatrix} \mathbf{K}(\mathbf{X},\mathbf{X}) + \nu^2 \mathbf{I}_{n_{\mathcal{D}}} & \mathbf{k}(\boldsymbol{z}^*,\mathbf{X}) \\ & \\ \mathbf{k}(\boldsymbol{z}^*,\mathbf{X})^{\top} & k(\boldsymbol{z}^*,\boldsymbol{z}^*) \end{bmatrix} \right) \tag{11}
$$

In this expression, the matrix function $\mathbf{K} : \mathcal{Z}^{1 \times n_{\mathcal{D}}} \times \mathcal{Z}^{1 \times n_{\mathcal{D}}} \to \mathbb{R}^{n_{\mathcal{D}} \times n_{\mathcal{D}}}$, is called the covariance or Gram matrix and is related to the kernel via $K_{j,l} = k(\boldsymbol{X}_{:,l}, \boldsymbol{X}_{:,j})$ for all $j, l \in \{1, \ldots, n_{\mathcal{D}}\}$.

The posterior predictive distribution of $f_{\text{GP}}(\boldsymbol{z}^*)$ is obtained by conditioning on the test point and the dataset $\mathcal{D}$, using Bayes' theorem:

225 $$\mathrm{p}(f_{\text{GP}}(\boldsymbol{z}^*)|\boldsymbol{z}^*,\mathcal{D}) = \frac{\mathrm{p}(f_{\text{GP}}(\boldsymbol{z}^*),\mathbf{Y}|\mathbf{X},\boldsymbol{z}^*)}{\mathrm{p}(\mathbf{Y}|\mathbf{X})} \tag{12}$$

The conditional posterior is a Gaussian distribution described by the mean and variance:

$$\mu(f_{\text{GP}}(\boldsymbol{z}^*)|\boldsymbol{z}^*,\mathcal{D}) = m(\boldsymbol{z}^*) + \mathbf{k}(\boldsymbol{z}^*,\mathbf{X})^{\top} \left(\mathbf{K}(\mathbf{X},\mathbf{X}) + \nu^2 \mathbf{I}_{n_{\mathcal{D}}} \right)^{-1} \left(\mathbf{Y} - [m(\boldsymbol{X}_{:,\mathbf{1}}), \ldots, m(\boldsymbol{X}_{:,\boldsymbol{n_{\mathcal{D}}}})]^{\top} \right) \tag{13}$$

$$\mathbb{V}\text{ar}(f_{\text{GP}}(\boldsymbol{z}^*)|\boldsymbol{z}^*,\mathcal{D}) = k(\boldsymbol{z}^*,\boldsymbol{z}^*) - \mathbf{k}(\boldsymbol{z}^*,\mathbf{X})^{\top} \left(\mathbf{K}(\mathbf{X},\mathbf{X}) + \nu^2 \mathbf{I}_{n_{\mathcal{D}}} \right)^{-1} \mathbf{k}(\boldsymbol{z}^*,\mathbf{X}) \tag{14}$$

A comprehensive detail of the derivation of these formulae can be found in Appendix A of Beckers (2021).

230 The prior mean function $m(\cdot)$ characterizes the average function under the GP distribution before any data is observed. This function presents a simple approach to include prior knowledge about the function we desire to model. An idealized physics model can hence be used as a prior. The GP then models the difference between this prior and the empirical data. When there is no such prior knowledge, a typical choice is to set the prior mean function to zero, i.e., $m(\cdot) \equiv 0$, but following our considerations about the physical climate response discussed in Section 2.3, we rather adopt an affine mean function of the

235 form

$$m(\boldsymbol{x}) = \beta_0 + \boldsymbol{\beta} \cdot \boldsymbol{x} + \beta_e \sqrt{x_1^2 + x_2^2} \tag{15}$$

where the last term accounts for a possible effect of the eccentricity. The coefficients β_i are chosen to minimize the sum of the squares of the residuals.

3.2 Application to climate fields

240 The regression approach discussed in the previous section is only applicable for sampling one-dimensional functions. However, when we model the GCM outcomes similarly to $\mathbf{f}_{\mathrm{GCM}}(\boldsymbol{z}) + \boldsymbol{\Sigma}$, we are confronted with a dimensionality challenge as the function's image is now of high dimension (a dimension equal to the number of grid points, or pixels). There are several strategies to manage this: using a Multi-Output Gaussian Process (MOGP) or an *outer-product* emulator (Rougier et al., 2009), creating a different GP for each dimension, and/or applying a dimensionality reduction technique (Wilkinson, 2010). Although

245 a MOGP could theoretically yield better results, its implementation for a GCM longitude-latitude grid is computationally challenging. The design of an appropriate kernel function would be highly complex, and the computational cost of GPR grows cubically with the number of samples ($\mathcal{O}(n_{\mathcal{D}}^3)$), making this approach impractical. In our study, we chose the third strategy and used Principal Component Analysis (PCA) as the dimensionality reduction technique. This choice was driven by our goal of preserving as many teleconnections within the data as possible. Constructing a different GP for each pixel would eliminate

250 many of these correlations. Moreover, the statistical interpretation of the principal components is advantageous, as they can be interpreted as either signal or noise. Furthermore, as the principal components are designed to be uncorrelated with each other, the use of a MOGP appears superfluous.

3.3 Kernel function

Equation 13 shows that the selection of the kernel function may significantly influence the posterior mean. The kernel is crucial

255 in expressing how the output associated with two neighbouring inputs are related. Hence, an inappropriate kernel choice or design can result in less accurate, or even incorrect, output (Rasmussen, 2006).

Selecting the appropriate function design with the correct number of hyperparameters is a complex task, but some studies offer an automated method for this search (Duvenaud et al., 2013). The most popular covariance function is the squared exponential kernel (SE-Kernel), as favoured by Kennedy and O'Hagan and Higdon et al. (2008).

260 In this study, we initially faced some issues when applying existing models to the Devonian dataset — only an unsatisfactory amount of the total variance could be emulated — and decided to search for a more general kernel function compared to Bounceur et al. (2015); Lord et al. (2017); Van Breedam et al. (2021). We settled to the work of Duvenaud et al. (2011) and employed an Additive Kernel, that presented slightly better performance. The kernel works as follows:

To each dimension $i \in \{1, \ldots, n_z\}$, we can assign a *base kernel* $k_i(\cdot, \cdot)$. An Additive Kernel is then the sum

265
$$k_{\mathrm{add}}(\boldsymbol{z}, \boldsymbol{z}') = \sum_{n=1}^{n_z} k_n(\boldsymbol{z}, \boldsymbol{z}') \tag{16}$$

where the first, second and n^{th} terms are given by

$$k_1(\boldsymbol{z}, \boldsymbol{z'}) = \sigma_1^2 \sum_{i=1}^{n_z} k_i(z_i, z_i') \tag{17}$$

$$k_2(\boldsymbol{z}, \boldsymbol{z'}) = \sigma_2^2 \sum_{i_1=1}^{n_z} \sum_{i_2=i_1+1}^{n_z} k_{i_1}(z_{i_1}, z_{i_1}') k_{i_2}(z_{i_2}, z_{i_2}') \tag{18}$$

$$k_n(\boldsymbol{z}, \boldsymbol{z'}) = \sigma_n^2 \sum_{1 \leq i_1 < i_2 < \cdots < i_n \leq n_z} \prod_{d=1}^{n} \tilde{k}_{i_d}(z_{i_d}, z_{i_d}') \tag{19}$$

where n_z is the dimension of the input space and $\sigma_n \in \mathbb{R}_0^+$. Specifically, the nth order interaction kernel k_n is the sum of $\binom{n_z}{n}$ terms. The relative magnitude of each σ_n informs about the importance of each order of interaction.

In this research, we have selected the Square Exponential Kernel (SE-Kernel) as the one-dimensional basis function:

$$\tilde{k}_{\text{SE}}(x, y; l) = \exp\left(-\frac{(x-y)^2}{2l^2}\right) \tag{20}$$

with $l \in \mathbb{R}_{>0}$ the lengthscale hyperparameter.

This kernel exhibits notable properties: it is stationary, meaning that it depends only on the distance between each point, and it is universal, implying that a GPR with such a kernel can approximate any continuous function with arbitrary precision on a compact set. Moreover, a SE-Kernel of high dimension can be seen as the product of multiple one-dimensional SE-Kernels.

The entire set of hyperparameters for the Additive Kernel is then defined by the $n_z = 4$ order variance $\{\sigma_1, \ldots, \sigma_{n_z}\}$ and lengthscales $\{l_1, \ldots, l_{n_z}\}$. These define a vector $\boldsymbol{\theta}$.

The first and last order terms in the sum are given by:

$$k_1(\boldsymbol{z}, \boldsymbol{z'}) = \sigma_1^2 \sum_{i=1}^{n_z} \exp\left(-\frac{(z_i - z_i')^2}{2l_i^2}\right) \tag{21}$$

$$k_{n_z}(\boldsymbol{z}, \boldsymbol{z'}) = \sigma_{n_z}^2 \exp\left(-\frac{1}{2} \sum_{i=1}^{n_z} \frac{(z_i - z_i')^2}{l_i^2}\right) \tag{22}$$

This Additive Kernel can be seen as an augmented SE-Kernel, as used in Lord et al. (2017). It maintains its properties and computational advantages while adding an optimal level of complexity. This complexity is enough to grasp useful information at a greater distance (see Fig 3), but still small enough to avoid over-fitting, classically known to appear when parameters to fit are too numerous.

3.4 Objective function and optimization

The GPR being non-parametric but the kernel function possess free parameters, known as hyperparameters, that must be optimized to best fit the data.

The negative log marginal likelihood function (Eq. 23), as fully derived in Rasmussen (2006), serves as an objective measure of model fit. It quantifies the likelihood of observing the given data under specific hyperparameters. The goal is to minimize this function to find the hyperparameters that maximize the model's likelihood of generating the observed data.
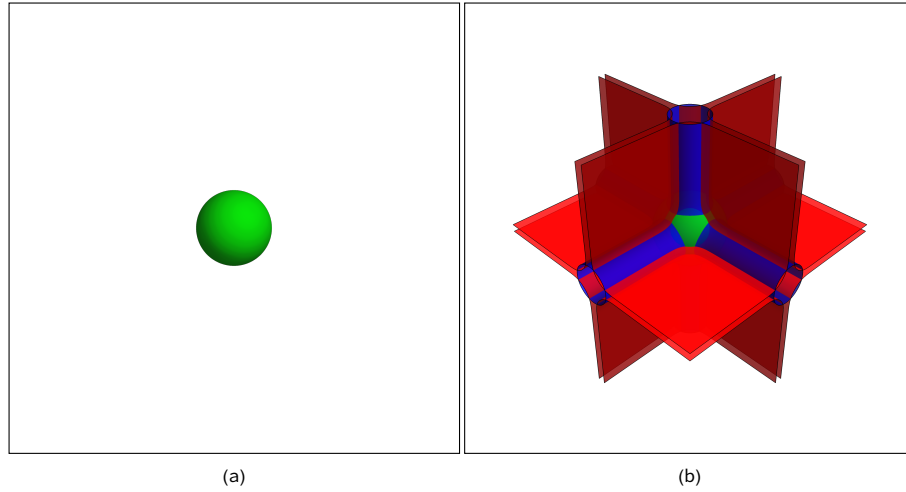
(a)   (b)

Figure 3. Isocontours of (a) a Square Exponential Kernel and (b) an Additive Kernel in a 3-dimensional space. The SE-Kernel is designed to give importance only to points in close proximity. In contrast, the lower-order kernels (in red and blue) are more inclusive. Reproduced from Duvenaud et al. (2011).

$$\log p(\mathbf{Y}|\mathbf{X},\boldsymbol{\theta}) = -\frac{1}{2}\tilde{\mathbf{Y}}^{\top}\left(\mathbf{K}(\mathbf{X},\mathbf{X};\boldsymbol{\theta})+\nu^2\mathbf{I}_{n_{\mathcal{D}}}\right)^{-1}\tilde{\mathbf{Y}} - \frac{1}{2}\log|\mathbf{K}(\mathbf{X},\mathbf{X};\boldsymbol{\theta})+\nu^2\mathbf{I}_{n_{\mathcal{D}}}| - \frac{1}{2}n_{\mathcal{D}}\log 2\pi \tag{23}$$

where we defined $\tilde{\mathbf{Y}} = \mathbf{Y} - [m(\boldsymbol{X}_{:,1}),\ldots,m(\boldsymbol{X}_{:,n_{\boldsymbol{D}}})]^{\top}$ to take into account a non-zero mean-function.

$$\begin{bmatrix}\boldsymbol{\theta}_{\text{opt}}\\ \nu_{\text{opt}}\end{bmatrix} = \arg\min_{\boldsymbol{\theta},\nu} -\log p(\mathbf{Y}|\mathbf{X},\boldsymbol{\theta}) \tag{24}$$

The negative log marginal likelihood function effectively balances model complexity and goodness of fit.

Optimizing the negative log marginal likelihood provides an approach to hyperparameter tuning with a theoretical justification. Furthermore, by design, it includes a complexity penalty that discourages overly complex models, effectively preventing overfitting and thus promoting the selection of parsimonious models.

Yet, its optimization can be computationally intensive, and complicated by the presence of multiple local optima.

With these difficulties in mind, we implemented the GPR in the Julia language using the versatile AbstractGP.jl package (Widmann et al., 2024) and Zygote.jl (Innes, 2019) to efficiently compute the gradients. The optimization scheme is based on the use of a bounded probabilistic descent and a local L-BFGS gradient descent algorithm, both made available within the Optimization.jl package (Dixit and Rackauckas, 2023). This method showed the best performance amongst other common algorithms. We initiate the algorithm from a wide range of initial conditions to ensure the achievement of a global minimum. Since the values to emulate are rescaled to be of order 1, we expect the lengthscale and order variance parameters to be of the same order. We first run 1024 optimizations at low tolerance from points lying in a Latin hypercube of bounds $[10^{-16}, 150]$

for each l_i, $[0, 2]$ for each σ_i and $[10^{-6}, 2]$ for ν^2 where a non-zero lower bound is present to ensure numerical stability. The 64 lowest different minima are kept and used in a second optimization round where the tolerance is set to a much lower value.

310 This algorithm almost guarantees that the final minimal value found is global.

A different objective function that was explored is the negative expected log pointwise predictive density (Gelman et al., 2014; Vehtari et al., 2017):

$$\log \mathrm{p}(y_{\mathrm{dat}}^{\{i\}}|\mathbf{X}, \mathbf{Y}_{-i}; \boldsymbol{\theta}) = -\frac{1}{2}\log \mathbb{V}\mathrm{ar}_{-i} - \frac{1}{2}\frac{\left(y_{\mathrm{dat}}^{\{i\}} - \mu_{-i}\right)^2}{\mathbb{V}\mathrm{ar}_{-i}} - \frac{1}{2}n_{\mathcal{D}}\log 2\pi \tag{25}$$

$$\mathrm{neldp}(\mathbf{X}, \mathbf{Y}; \boldsymbol{\theta}) = -\sum_{i=1}^{n_{\mathcal{D}}} \log \mathrm{p}(y_{\mathrm{dat}}^{\{i\}}|\mathbf{X}, \mathbf{Y}_{-i}; \boldsymbol{\theta}) \tag{26}$$

315

$$\begin{bmatrix} \boldsymbol{\theta}_{\mathrm{opt}} \\ \nu_{\mathrm{opt}} \end{bmatrix} = \arg\min_{\boldsymbol{\theta}, \nu} \mathrm{neldp}(\mathbf{X}, \mathbf{Y}; \boldsymbol{\theta}) \tag{27}$$

where μ_{-i} and $\mathbb{V}\mathrm{ar}_{-i}$ are computed according to Eqs. 13 and 14 while removing the point $\{\boldsymbol{x}_{\mathrm{dat}}^{\{i\}}, y_{\mathrm{dat}}^{\{i\}}\}$. While this approach excels in identifying the optimal representation of the dataset, it is hindered by its slow speed due to its computational complexity, which also significantly complicates the use of automatic differentiation. Therefore, we decided to not use this method

320 in our study and instead focus on the negative log marginal likelihood function.

3.5 Data preprocessing

As discussed in Section 3.2, the GPR is not directly applied to the climate fields but rather to the PCA loading coefficients, building an independent GP for each component. PCA condenses the variability of multivariate observations into a set of orthogonal modes, known as principal components (PCs). These PCs encapsulate the most significant patterns in the data. The

325 mathematical foundation of PCA involves the computation of eigenvalues and eigenvectors from the data's covariance matrix. The eigenvectors, also termed as loadings, signify the directions of maximum variance, while the eigenvalues quantify the variance explained along each eigenvector. These loadings offer insights into the relationships amongst the original variables and assist in identifying the primary modes of variability within the dataset.

The decomposition of the output in PCs is a linear operation (although the PCs themselves are non-linear), as illustrated by

330 the following equations:

$$\boldsymbol{y} = \mathbf{P}_{\mathrm{GCM}}^{\top}(\boldsymbol{x} - \boldsymbol{\mu}_{\mathrm{GCM}}) \tag{28}$$

$$\tilde{\boldsymbol{x}} = \mathbf{P}_{\mathrm{GCM}}\boldsymbol{y} + \boldsymbol{\mu}_{\mathrm{GCM}} \tag{29}$$

In Eq. 28, $\mathbf{P}_{\mathrm{GCM}}$ denotes the matrix of loadings, whose columns are the orthonormal eigenvectors of the data. The term $\boldsymbol{x}$ signifies a climate field that has been reshaped into a vector and imputed for missing values, while $\boldsymbol{\mu}_{\mathrm{GCM}}$ represents the mean

335   value of each grid cell, also reshaped into a vector. The term $\boldsymbol{y}$ is the projection of $\boldsymbol{x}$ onto the lower-dimensional vector space spanned by the PCs, the components of $\boldsymbol{y}$ are often referred to as the PCA scores. These scores are the scalar values interpolated using the GPR.

Eq. 29 demonstrates how to reconstruct the climate field from the lower-dimensional representation (denoted by $\tilde{\boldsymbol{x}}$). This reconstruction is approximate and will only be exact if the true value $\boldsymbol{x}$ resides within the vector space spanned by the data

340   used to generate the projection matrix. This equation is employed to reconstruct the GCM outcomes using the results from the GPR.

For optimal performance of PCA, certain data assumptions must be satisfied. Specifically, the data should follow a Gaussian distribution to ensure the validity of statistical measures like covariance. Standardizing (i.e., subtracting the mean and dividing by the standard deviation) is also a common procedure for ensuring comparability in scale across pixels, preventing dominance

345   by points with larger magnitudes.

Standardization of each pixel is typically applied to data that follows a Gaussian distribution which is the case for our temperature data. Precipitation minus evaporation (or *runoff*, which often contains many zeros in arid grid cells) is conversely highly asymmetric and skewed. In that case, standardization does not yield a Gaussian distribution via affine transformation of the data.

350   In this study, we chose to standardize temperature but not runoff before computing the PCA. This is the approach that proved to be the most effective. Additionally, we opted to emulate the total annual water volume (i.e., runoff multiplied by area) rather than runoff directly. This decision is motivated by the unequal areas of grid cells. As a result, this procedure effectively assigns greater weight to tropical regions, which are of particular interest in our study.

The PCA scores themselves are also rescaled. Indeed, the magnitude of these scores is proportional to $\sqrt{\lambda}$, where λ is the

355   variance associated with the principal component of interest (i.e., an eigenvalue). To ensure the stability of the optimization algorithm and the interpretability of the objective function, we divide each coefficient by $2\sqrt{\lambda}$. This transformation ensures that the values to be interpolated typically lie between -1 and 1 and have the same scale across different principal components.

In principle, some experiments may exhibit a highly non-linear behaviour, e.g. by crossing some tipping points, and effectively behave as outliers. When the occur they deserve particular attention because they may complicate the learning process

360   and justify a specific treatment.

The adopted strategy to detect these points is based on the PCA decomposition of the set. We assume that each component of $\boldsymbol{y}$ follows a Gaussian distribution. The mean and standard deviation of each principal component are computed while excluding a specific GCM outcome. This outcome is then projected onto the lower-dimensional vectorial space spanned by the remaining data, and its z-score is computed as follows:

365
$$z_{\text{score},k} = \left| \frac{\tilde{y}_k^{\{i\}} - \mu_k^{\{-i\}}}{\sigma_k^{\{-i\}}} \right| \tag{30}$$

Here, the superscript $\{i\}$ is the experiment index, $\{-i\}$ signifies that μ and σ have been computed excluding the specific experiment, and the subscript k is the PC dimension. If the value of this score is higher than a specific threshold (e.g., 3 for a 99.73% accuracy) for the main contributing PCs, then the probability that the behaviour of this GCM run is an outlier is

high and should be excluded, or at least specifically examined. In our set of 81 HadSM3 runs, though, none of them had to be
370   excluded and no specific treatment was thus necessary.

3.6   Validation

The last step in our process is to determine the best number of PCs to emulate. Insufficient PCs could result in information loss, while an excess might introduce noise, given that the least significant components often resemble random fields attributable to the GCM internal variability.

375   In this study, we opted for a dimensionless metric: the weighted Concordance Correlation Coefficient (CCC) (Lin, 1989), to quantify the accuracy of emulator-based reconstructions.

$$\rho_c(\boldsymbol{y},\hat{\boldsymbol{y}}) = \frac{2\sum_i w_i(y_i - \mu_y)(\hat{y}_i - \hat{\mu}_y)}{\sum_i w_i(y_i - \mu_y)^2 + \sum_i w_i(\hat{y}_i - \hat{\mu}_y)^2 + (\mu_y - \hat{\mu}_y)^2} \tag{31}$$

where $\hat{y}_i$ denotes the prediction, and y_i the GCM output. This approach involves excluding a single data point during training and using it to validate the emulator's prediction. The calculated CCC values, combined with the loss function, guide the se-
380   lection of the optimal number of PCs to retain for each variable.

As indicated by Figure 4, retaining the first 7 PCs for both runoff and surface temperature achieves an effective balance between minimizing information loss and avoiding noise amplification. This compromise ensures the emulator's robustness and reliability for climate field predictions.

385

We can also use the same metric to evaluate the effectiveness of a more complex kernel function. To do so, we compare two emulators designed to be as similar as possible; their only difference lies in the correlation function $k(\boldsymbol{z},\boldsymbol{z}')$. For one emulator, this function is an *Additive Kernel* as described earlier, while for the other it is the more conventional *Square Exponential kernel*, as used in previous studies (Bounceur et al., 2015; Lord et al., 2017; Van Breedam et al., 2021). Figure 5 presents
390   the results of this comparison for continental runoff – the variable that initially motivated the development of this improved emulator because of its initial poor predictability. We observe that employing the Additive Kernel function results in superior performance for almost all the test experiments.

3.7   Interpretation and sensitivity

Figure 6 shows the first six PCs and the associated normalized variance $\lambda_i/\lambda_{\text{tot}}$, which indicates the proportion of variability
395   each PC explains. As these are variations relative to the mean value and can be multiplied by either a positive or negative factor, the sign is not inherently meaningful. Consequently, the terms 'cooling' and 'warming' can be interchanged without loss of generality in the subsequent discussion.

    The first PC, accounting for approximately 97% of the total variance, represents a global anomaly, where the sign is consistent across locations, but the intensity varies. As inferred from Figure 7 (a), this component primarily results from changes in
400   $p\mathrm{CO}_2$. However, as depicted in 8 (a), eccentricity has a similar signature, as expected, since this parameter modulates the total
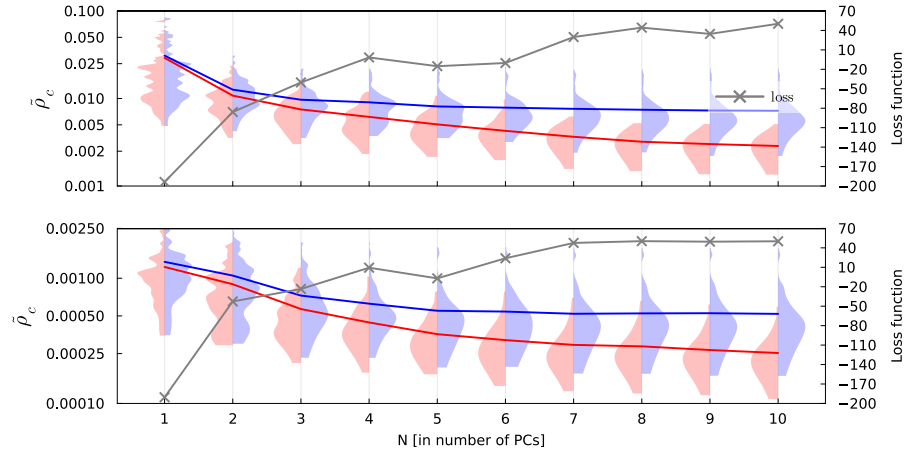
15

Figure 4. Shifted concordance correlation coefficient ($\tilde{\rho}_c = 1 - \rho_c$) distributions (left axis, in log-scale) and individual loss function value (right axis) for runoff (top) and surface temperature (bottom). In blue, the CCC has been computed on a sample while having excluded it during the learning process (*leave-one-out*; LOO). In red are depicted the CCC using the full set of experiments. Plain blue and red lines represent the average value across the whole set of 81 GCM runs, while the grey line indicates the objective function value for the specific N^{th} PC.
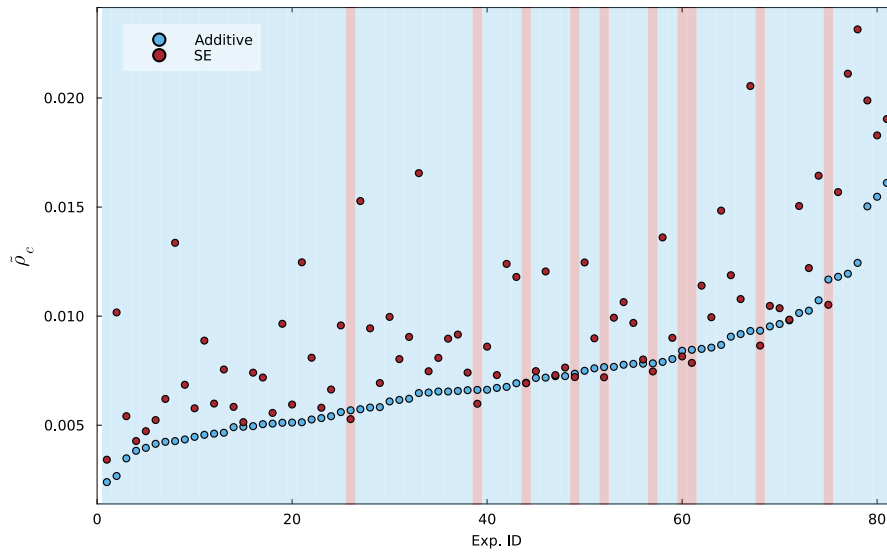
Figure 5. Comparison of the performance of the two kernel functions: Additive and Square Exponential (SE). Each point represents the shifted CCC value computed between the GCM climate field and the prediction produced by an emulator trained on the dataset with the specific experiment omitted (LOO). A blue background indicates that the Additive Kernel outperforms the alternative in that experiment, whereas a red background signifies that the SE kernel achieves better performance. The 81 experiments were sorted by $\tilde{\rho}_{c,\text{Additive}}$ for clarity.

amount of radiation received from the Sun. The second PC depicts a polar effect, with cooling at the poles and warming in the mid-latitudes. As shown in Figure 7 (b), this effect is mostly attributable to changes in obliquity.

The subsequent PCs reveal more localized variations. Notably, the sixth PC is highly localized and shows most of its effect in the polar south region. This specific temperature anomaly can be attributed to the presence of sea ice. To capture this particular

405 pattern, it may be beneficial to design a focused emulation process for this region. This approach would increase the variance of this specific component, enabling better handling by the GPR. Visualization of the remaining PCs shows that this particular area is the only one with a significant anomaly, suggesting that the other PCs are less relevant for the emulation process. A specific design where different GPRs are trained for continental and sea-surface temperature has also been considered, but the performance improvement – it showed slightly better results amongst 55% of the training set – was not deemed significant

410 enough to justify the additional computational cost when merged inside GEOCLIM.

As described in the previous text, most of the variance arises from changes in pCO_2. Indeed, the experimental design allows for significantly more variance in this direction than in climate precession. However, one could restrict the parameter space accordingly and compute, for instance, the global mean surface temperature (GMST) to test whether the results are consistent with the astronomical forcing or not. If we assume that a doubling of CO_2 decreases outgoing radiation by $3.7\,\mathrm{W\,m^{-2}}$, and that

415 the transition from zero eccentricity to $e_{\max}$ is equivalent (in terms of total mean annual radiative forcing) to (Milankovitch, 1941; Berger and Loutre, 1994):

$$\left(\left(1 - e_{\max}^2\right)^{-\frac{1}{2}} - 1\right)\frac{S}{4} \approx 0.93\,\mathrm{W\,m^{-2}}$$

for $e_{\max} = 0.075$ and $S = 1322\,\mathrm{W\,m^{-2}}$, then we can estimate that a multiplicative factor of $2^{\frac{1.06}{3.7}} \approx 1.2$ for pCO_2 would produce similar effects on GSMT for both astronomical forcing and carbon dioxide.

420

As shown in Figure 9, a 20% variation in pCO_2 results in a GMST change equivalent to the effect of increasing eccentricity from $e = 0$ to $e = 0.075$, corresponding to approximately $+0.7\,°C$. This suggests that orbital variability is not overshadowed by variations in atmospheric carbon dioxide.

3.8 Coupling to GEOCLIM

425 The GP calibration is done in a high-level computing language, namely Julia, for easier tuning and understanding of the code. However, most of the historical models in climate science are written in Fortran, and this is the case for GEOCLIM. Once trained, making a prediction with the emulator boils down to multiplying matrices, operations that are well optimized in Fortran using the OpenBLAS library. A script to automatically generate the Fortran routine, given a trained emulator, has been written for this coupling purpose.

430 In our setup, we want the pCO_2 to be interactive and, therefore, cannot precompute the whole climate time series, as we need input from the biogeochemical model to predict the next climate state. The coupling time is an arbitrary parameter that depends on the time resolution desired and the magnitude of climatic perturbations. Depending on the situation, this parameter can be easily adjusted to a different value. Given the processes featured by GEOCLIM and the timescale of astronomical forcing, it is
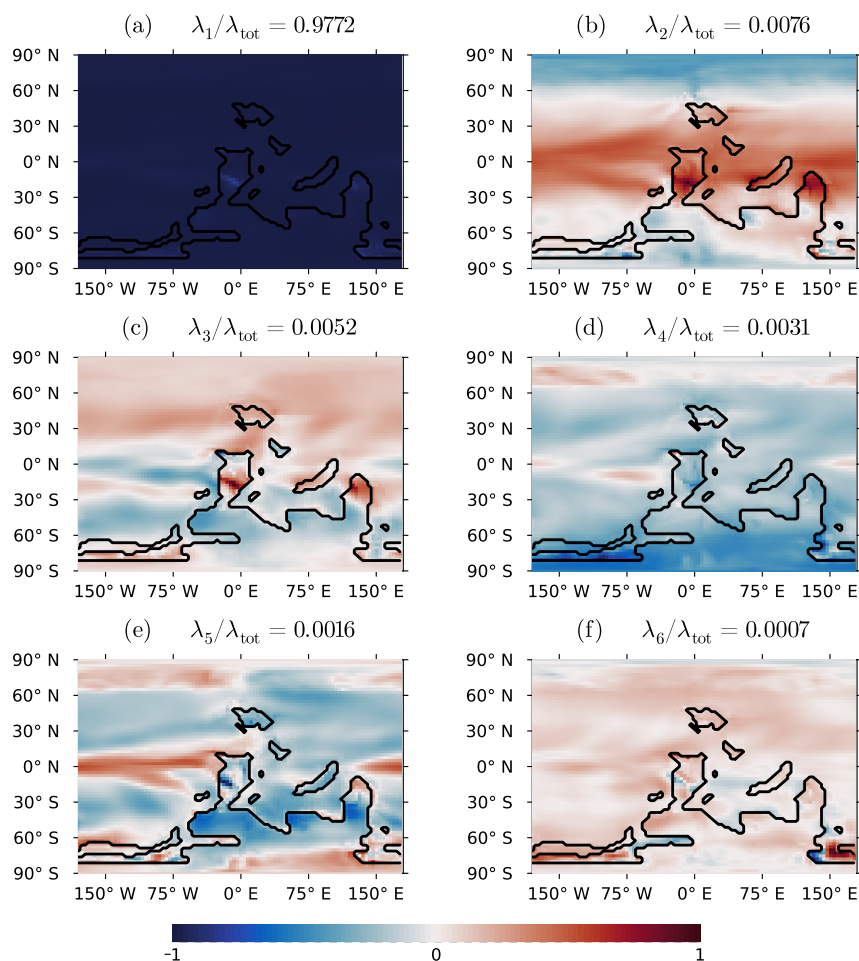
Figure 6. The figure presents the first six principal components of the surface temperature, ordered by their eigenvalues and rescaled by a multiplicative factor. The colour scale is indicative of the amplitude and its sign within a single PC, but is independent across different PCs. The black lines delineate the coastlines of the continental configuration.

conservative to update the climate fields every 25 years and synchronize it with the calls of the continental weathering module. We do not expect any process to operate on a faster timescale.

4 Case study: orbital forcing of the Late Devonian climate

4.1 Calibration of GEOCLIM

GEOCLIM version 6.1.0 was selected for long-term carbon cycle modelling. While the primary modification is the implementation of the emulator for dynamic climate computation, several other adjustments were necessary for our model setup.
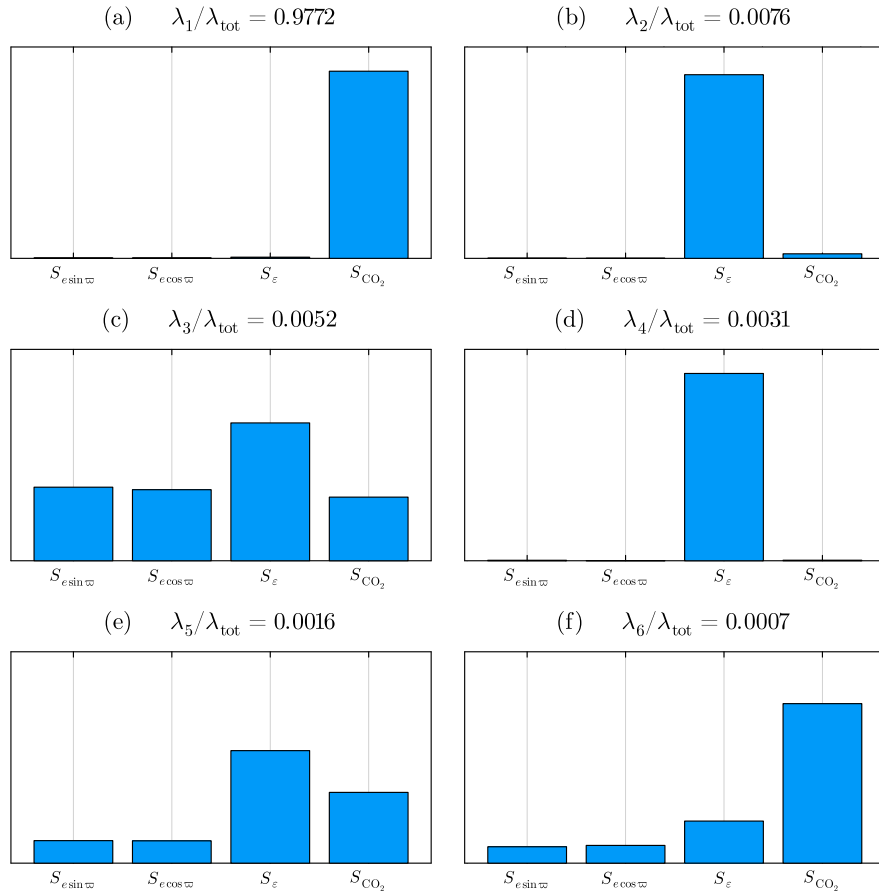
Figure 7. Magnitudes of the total Sobol index for each input variable. A superior total-order Sobol index signifies the parameter's comprehensive influence on the output's variability, integrating both direct impacts and interaction effects. Due to a larger domain explored for the carbon dioxide and obliquity, the effect of climatic precession is screened (c.f. Figure 8).

440   The temperature of each oceanic box is determined through a linear relationship with the global sea-surface temperature (GSST):

$$T_i = \gamma_{0,i} + \gamma_{1,i} \times \text{GSST} \tag{32}$$

where the GSST is derived from the emulator output. The coefficient vectors γ were fitted using least-squares regression on a set of cGENIE simulations that employed a similar continental configuration (Gérard et al., 2025). These simulations followed
445   the same experimental design as our 81 HadSM3 runs. Water mass exchanges between neighbouring boxes were also updated accordingly, though kept constant in time and across experiments as this version of GEOCLIM is not designed to include a dynamic ocean circulation.
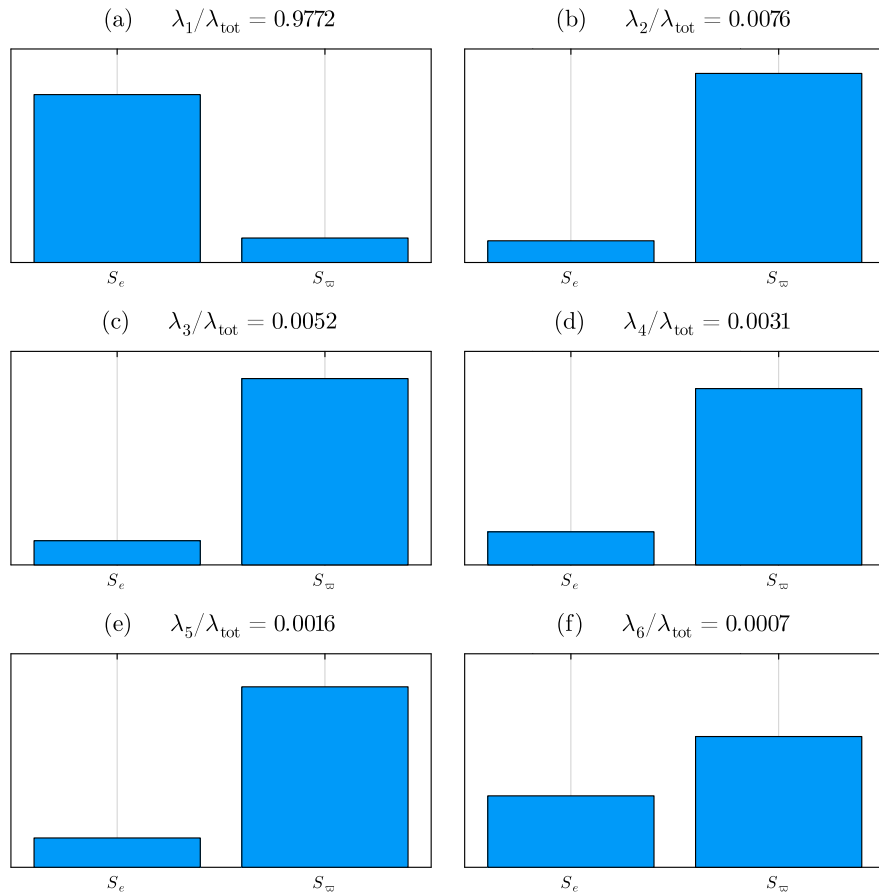
Figure 8. Magnitudes of the total Sobol index for eccentricity e and longitude of the perihelion ϖ. To obtain this figure, the values of obliquity and pCO_2 were held constant respectively at $\varepsilon = 22.23°$ and 5×280 ppm.

Following the methodology outlined in the supplementary material of Maffre et al. (2021), we calibrated the uncertain parameters using a present-day configuration. Box geometries (volumes and surfaces) were computed using Scotese's recon-
450   struction. The surfaces and volumes of epicontinental boxes, which carry significant uncertainty, were adjusted to achieve an equilibrium concentration of $10 \, \mathrm{mol \, m^{-3}}$ dissolved SO_4 in the ocean (Cai et al., 2022), using mean-orbital parameters ($e = 0$ and $\varepsilon = 22.23°$).

Given the substantial uncertainties in reconstructing solid Earth degassing rates during the Devonian period (Marcilly et al., 2021; Müller et al., 2024), we adopted a fixed value in this study. This value was determined by calculating the degassing
455   rate necessary to balance the total silicate weathering consumption in a present-day configuration, corresponding to the rate required to maintain a steady atmospheric pCO_2 level of 280 ppm.
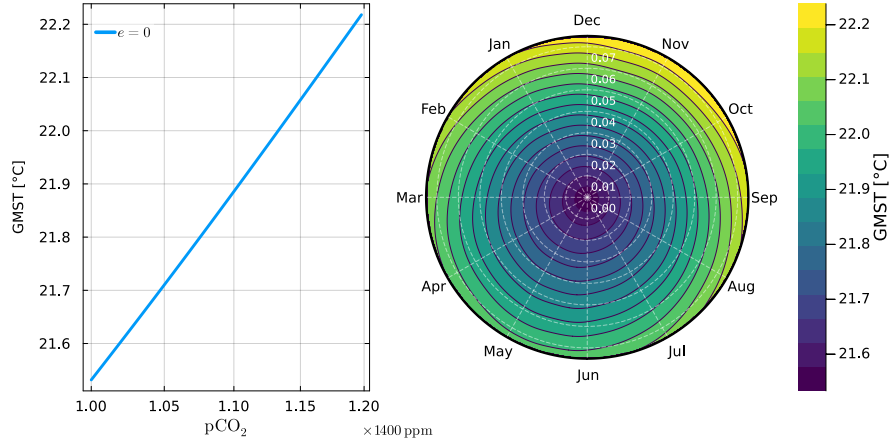
Figure 9. The left panel shows the global mean surface temperature (GMST) for a fixed astronomical configuration ($e = 0$, $\varepsilon = 22.23°$) with pCO_2 varying from 5×280 ppm to $1.2 \times 5 \times 280$ ppm. On the right is displayed a phase contour plot of the GMST, with the eccentricity as the radius and the longitude of perihelion as the azimuthal angle. The angle is expressed in the month when the Earth is closest to the Sun, such that the vertical axis is the climatic precession $e \sin \varpi$ and the horizontal axis is the coprecession $e \cos \varpi$. The polar representation is shown for a fixed obliquity ($\varepsilon = 22.23°$) and a constant pCO_2 of 5×280 ppm.

4.2 Fourier analysis of the response

The development of this emulator and modelling strategy was motivated by investigating the potential connection between astronomical forcing and the timing of Devonian OAEs, as discussed in the introduction. Previous studies by De Vleeschouwer
460 et al. (2024), and Wichern et al. (2024) hypothesized that reduced seasonal contrasts during eccentricity minima within 2.4 Myr nodes facilitate gradual regolith accumulation on continents. This accumulated regolith is subsequently mobilized and eroded during the first pronounced precession maximum following the node. Our modelling framework enables the investigation of potential long-term effects within geological soil systems.

In this part, we present an integrated result of the emulator into GEOCLIM6.1.0. The astronomical scenario, which outlines
465 the values of the three orbital parameters over time, is a plausible but hypothetical scenario, given that no precise solution for the Devonian can be produced. We use the planetary solution La10a provided by Laskar et al. (2011a), and selected the period $125 - 100$ Ma, during which 2.4 Myr eccentricity nodes are well-marked. We coupled this solution with the precession model of Sharaf and Boudnikova (1967), following the procedure outlined in Berger and Loutre (1991). This procedure implies, first, a harmonic decomposition of the planetary solution (using R-code based on Šidlichovský and Nesvorný (1997)) and then
470 specification of reference obliquity and general precession rate. The latter are given by Farhat et al. (2022) for the period of 370 Ma. With this construction, the solution has obliquity frequencies of 30555 and 37335 years, and climatic precession frequencies of 16470 and 19386 years considered to be plausible for the Devonian. The R-code used to generate those time series is available in Crucifix (2025).
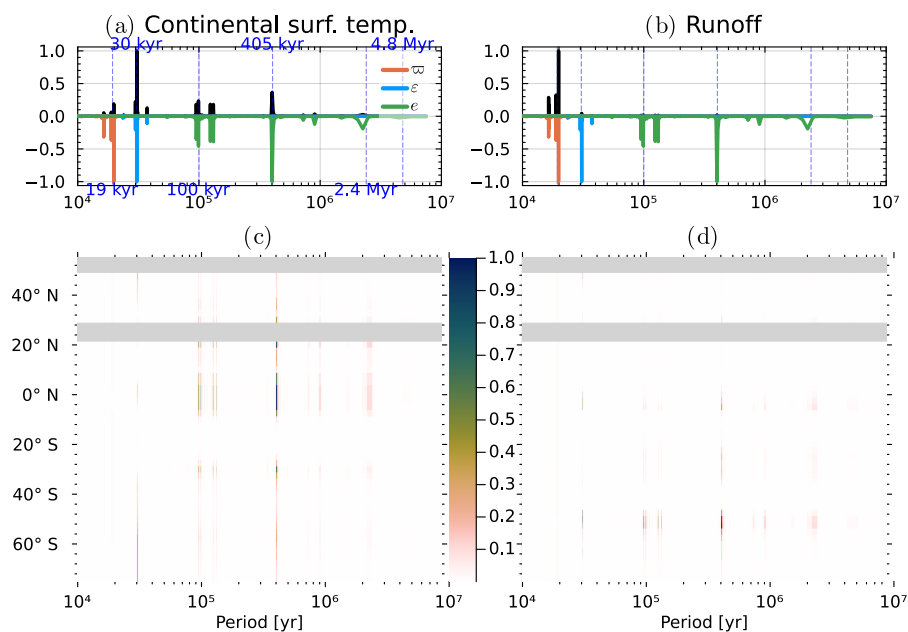
21

Figure 10. Normalized Fourier power spectral density of (a) & (c) continental surface temperature and (b) & (d) runoff. The top panels show the spectrum of the spatial average in black and the spectra of the orbital parameters flipped over the x-axis (for a better visibility) and the bottom panels display the latitudinal averages. Various important cycles are shown in vertical dashed blue lines as landmarks.

Starting from its calibration value, the model was run for 25 Myr. The last 22.5 Myr were selected for detailed analysis
475   because the static equilibrium state, which has a slightly higher pCO_2, differs from the dynamic equilibrium state. The initial 2.5 Myr were used to stabilize the model and avoid an unwanted artifact trend.

Figure 10 shows the normalized Fourier power spectral density of the forcing (i.e., the three orbital parameters) and of a spatial average and latitudinal band of the climate fields, specifically continental temperature and runoff. These fields are internally computed by the emulator based on the orbital parameters and carbon dioxide concentration. Globally, the surface
480   temperature shows a strong influence from the obliquity and eccentricity cycles. Conversely, runoff is primarily affected by climatic precession ($e \sin \varpi$). Locally, the long eccentricity cycle (± 405 kyr) seems to be dominant, but its influence is reduced when considering the global average. The 2.4 Myr cycle is present in the forcing, but its influence on the climatic fields is very weak.

From Figure 11 (a) & (c), we can observe that the atmospheric pCO_2 and average regolith thickness exhibits strong 405
485   kyr and 2.4 Myr cycles, suggesting the presence of a long-term response in the subsystem. As depicted in Figure 12, the amplification of the 2.4 Myr cycle is a spatially localized feature, with a maximal amplitude around the tropics. Time series of GEOCLIM outputs are presented in the following section to further investigate this local phenomenon. However, these cycles are almost absent from the total reactive phosphorus flux, as shown in Figure 11 (b). Under the parametrization of GEOCLIM, this result is inconsistent with the hypothesis that the regolith thickness is the main driver of the nutrient weathering flux.
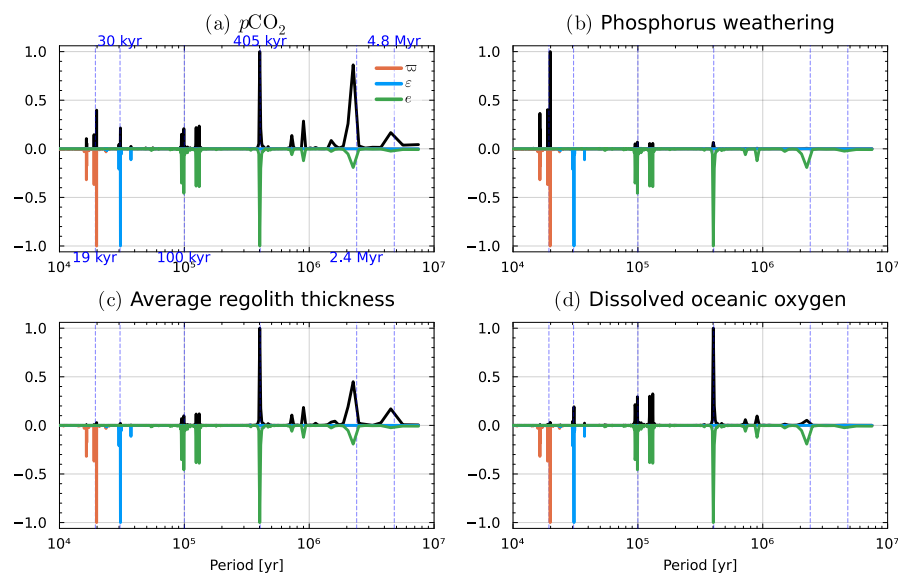
22

Figure 11. Normalized Fourier power spectral density of (a) atmospheric pCO_2, (b) total reactive phosphorus weathering flux, (c) global average regolith thickness and (d) global oceanic dissolved oxygen. The spectra of the orbital parameters are shown flipped over the x-axis. Various important cycles are shown in vertical dashed blue lines as landmarks.
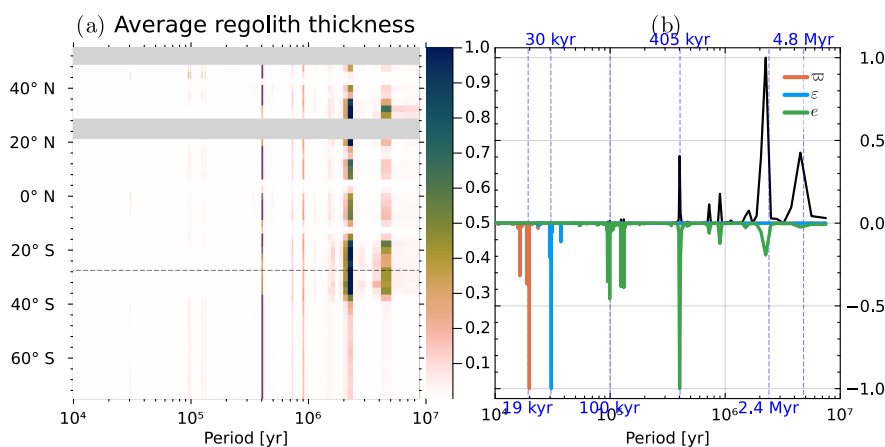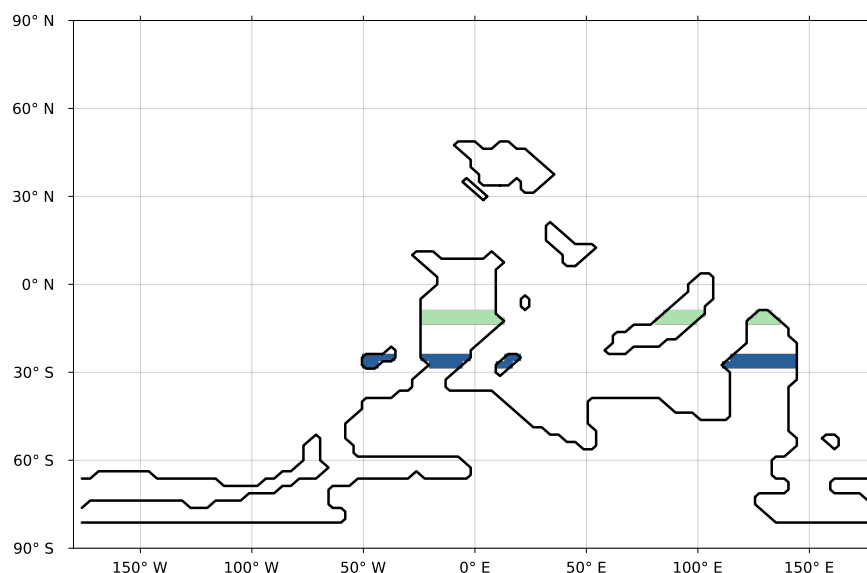

Figure 12. Normalized Fourier power spectral density of (a) longitudinal average of the regolith thickness and (b) a section at $27.5°$ S, represented by the dashed line in (a). The spectra of the orbital parameters are shown flipped over the x-axis. Various important cycles are shown in vertical dashed blue lines as landmarks.

Figure 13. The two regions under consideration for the spatial averages in Figure 14. The green region is consistently wet, while the blue region, located at the edge of the intertropical convergence zone (ITCZ), can experience arid conditions under precession minima.

4.3 Regolith dynamics

Here, we examine the variations in regolith thickness within the model. Regolith thickness is a crucial parameter in GEOCLIM, controlling weathering rates and serving as the closest proxy for a continental nutrient reservoir. As such, it is central to many hypotheses regarding Devonian OAEs.

The simulation employs the same astronomical scenario as previously described, but with obliquity held constant at 22.23° to isolate the effects of eccentricity and climatic precession. Figure 14 presents a 2 Myr segment of this scenario, displaying three model outcomes: atmospheric carbon dioxide concentration, average runoff, and surface temperature in two distinct regions illustrated in Figure 13.

Figure 14 shows a clear precession signal on the runoff and surface temperatures. Nonetheless, the amplitude and duration of these perturbations alone are insufficient to independently trigger a global OAE. As depicted in Figure 15, the regolith in the green region predominantly maintains equilibrium and does not exhibit significant thickening paced by eccentricity. Conversely, the blue region demonstrates growth paced by this parameter. The green region can be characterized as an ever-wet tropical region, whereas the blue region experiences aridity paced by precession minimum.

In the blue region, when eccentricity is high, the moisture available during a precession maximum amplifies regolith production more than it augments erosion, resulting in a thickening of the regolith. In the ensuing precession minimum, the absence of water for production or erosion renders the regolith static until the next precession maximum for further growth. This mechanism operates as long as the eccentricity increases. However, under conditions of decreasing eccentricity, the subsequent
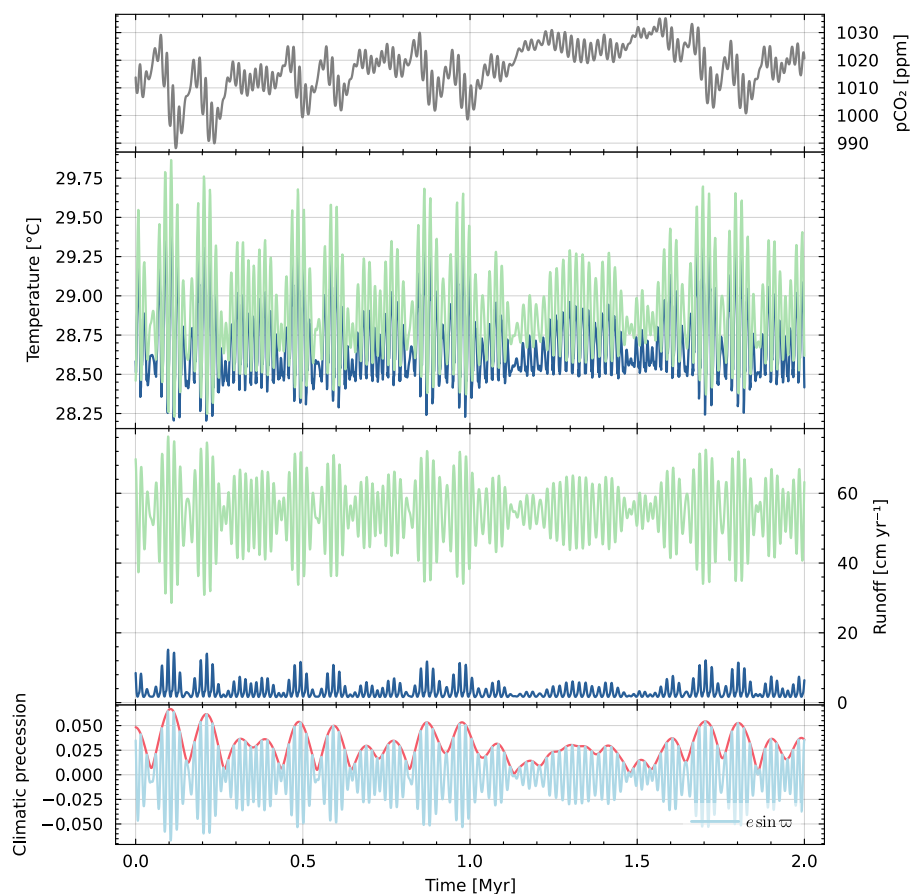
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Figure 14. This figure displays a 2 Myr long segment of a plausible Devonian orbital solution with constant obliquity. The top line represents the atmospheric $p\mathrm{CO_2}$, the blue and green curves are spatial averages on the respective regions of the same colour as depicted in Figure 13. The eccentricity is shown in red on the bottom graph. Except for climatic precession, which is the forcing here, all other curves are outcomes of the model. This section has been chosen to specifically show a 2.4 node, approximately located between 1.1 and 1.5 Myr, where the 100 kyr eccentricity signal is almost absent.

precession maximum lacks sufficient wetness to sustain the thickness of the regolith, leading to production becoming lower than erosion. A remarkable phenomenon can be observed during an eccentricity node. During this period, the eccentricity is low for a complete 405 kyr cycle, and the regolith thickness at the beginning, resulting from previous high eccentricity cycles, is more important than its equilibrium value. This results in a significant higher erosion than production of the regolith during the node, creating an important 2.4 Myr cycle in the signal thickness.

In the green region, both production and erosion are influenced to a comparable degree by precession, resulting in the regolith nearing a steady-state.
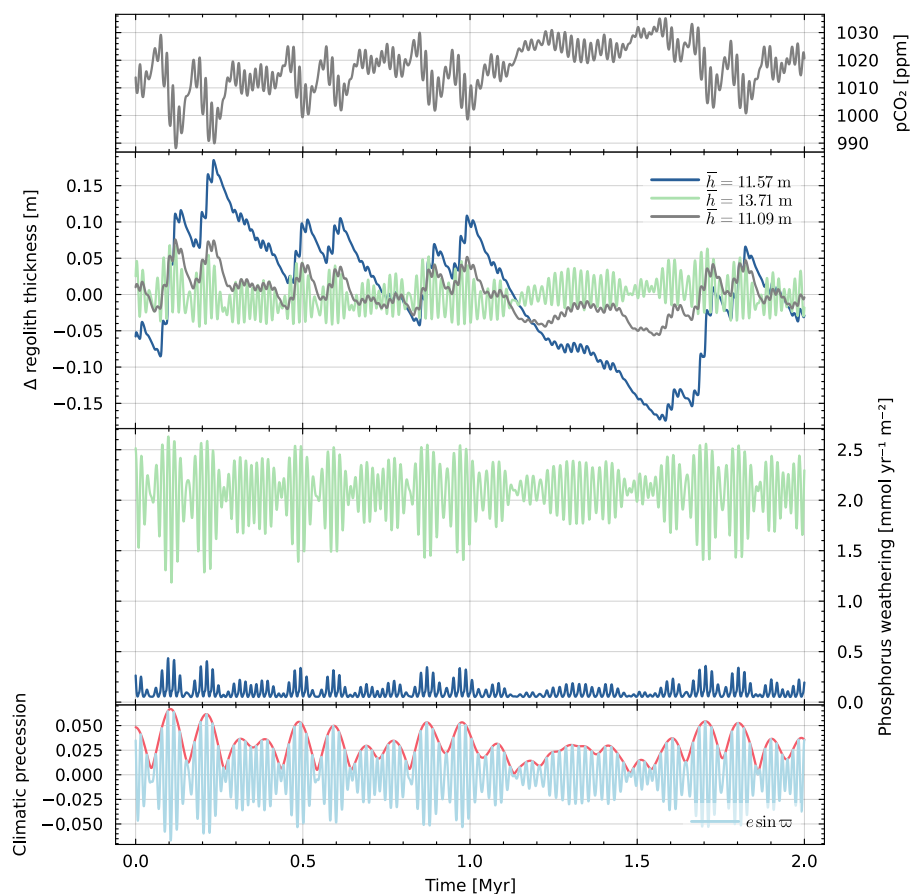
25

Figure 15. Displayed alongside the pCO_2 and orbital forcing are the average regolith thickness variation with respect to the temporal mean $\bar{h}$ and phosphorus weathering, following the colour convention for each region defined in Figure 13. The third grey line of the second panel depicts the global behaviour of the regolith thickness variation.

From these findings, our model suggests an alternative narrative to the eccentricity node hypothesis. Globally, the regolith (functioning as a nutrient reservoir) demonstrates a positive correlation with eccentricity, indicating that soil development occurs predominantly during high eccentricity periods rather than during nodes. Furthermore, the impact of regolith thickness variations on oceanic nutrient fluxes appears minimal.

As illustrated in Figure 15, these variations are relatively modest, with runoff – primarily controlled by climatic precession $e\sin\varpi$ – emerging as the dominant driver of weathering and erosion processes. Moreover, the majority of nutrients originate from regions analogous to the green zone, where significant long-term response effects appear absent.

4.4 Discussion of the case study

With this case study, we now have a framework for studying the astronomical forcing on regolith dynamics during the Devonian period. With the hypotheses adopted here (fixed palaeography, solid Earth degassing, vegetation and constant lithology), results indicate that regolith build-up is more closely linked to periods of high eccentricity rather than to eccentricity nodes.

525 More specifically, we found that climatic precession ($e \sin \varpi$) primarily controls runoff and weathering, while the direct impact of regolith dynamics on nutrient fluxes appears minimal. This confirms that, in the Devonian context, additional environmental factors are necessary to trigger widespread OAEs. For example, obliquity may play a role in sea-level variation through effects from ice sheets (Ma et al., 2022, 2025). While no strong conclusions regarding the precise timing and pacing of anoxic events can be drawn from these results due to the relatively small amplitude of the simulated dissolved oxygen vari-

530 ations and the model design, we have established a solid basis for exploring the dynamics of Devonian anoxia. Future work directions should include vegetation feedbacks and an improved ocean discretization (Algeo and Scheckler, 2010; Maffre et al., 2022; Smart et al., 2023; Maffre et al., 2024).

5 Conclusions

In this study, we presented a dynamically coupled Gaussian Process emulator designed to bridge the gap between complex

535 General Circulation Models and geochemical simulations over geological timescales. Our approach leverages an optimized training dataset, advanced kernel functions, and robust hyperparameter tuning to capture essential climate dynamics while significantly reducing computational costs. The additive kernel framework, inspired by Duvenaud et al. (2011), allowed us to account for both individual and interacting effects of key input parameters, and the integration of PCA ensured that the emulator maintained crucial spatial teleconnections. Furthermore, the development of the emulator has taken into account the

540 importance of a careful treatment of the Anomalous Heat Convergence flux to avoid possible global unwanted parameter-dependent forcing, and has underscored that Principal Component Analysis is effective for dimensionality reduction while a specific pre-processing of the input variables can slightly impact the emulator's performance.

The proposed method not only reproduces key features observed in the HadSM3 simulations but also provides a flexible tool for exploring the parameter space robustly and efficiently. As a case study, the setup has been applied to a 25 Myr Devonian

545 orbital scenario to test the relationship between orbital forcing, regolith dynamics and nutrient fluxes. Our preliminary findings indicate that high eccentricity, rather than low eccentricity, promotes regolith growth, though the variations are not significant enough to have a substantial impact on the nutrient fluxes. Therefore, it is very challenging to produce an OAE by the effect of astronomical forcing only on the atmospheric components in this setup.

By enabling the investigation of multiple astronomical scenarios at minimal computational cost, our emulator provides

550 valuable insights into the complex relationship between orbital forcing and palaeoenvironmental changes.

Our application on the Devonian shows that we have a modelling framework stimulating research directions for understanding the mechanisms of anoxia during that period. Yet, the methodology is also applicable to other geological intervals throughout the Phanerozoic. More generally, it contributes to addressing the crucial challenge of studying Earth's climate sys-

tem across a wide range of timescales in biogeochemical models, from yearly variations to million-year-long geochemical
555 processes. We believe this work lays a solid foundation for enhancing our understanding of palaeoenvironmental variations
and their driving mechanisms across the Phanerozoic.

Appendix A: Anomalous heat convergence

In a slab model, the atmosphere is coupled to a much simpler resolution of the ocean, having a single layer. This coupling has the advantage of still capturing the first order interaction of the ocean without the need of running experiments for several thousands of years, as the response is much faster. However, the model must be calibrated on realistic ocean to be able to capture its dynamic.

In this work, we performed 15 experiments using HadCM3, changing only the three orbital parameters (see Figure A2). After 250 years, the upper layer of the ocean was close to equilibrium, and the simulation was stopped (the deep ocean could take more than 3000 years of model run). The obtained SST and sea-ice concentration fields were then prescribed to the slab model to diagnose the Anomalous Heat Convergence (AHC).

The anomalous heat convergence refers to the term in the thermodynamic equation that represents the imbalance between the incoming and outgoing energy fluxes at a specific point within the model. In slab models such as HadSM3, it is used as a monthly forcing to best represent the first order atmosphere-ocean interaction.

At steady state, the temporal and spatial mean of the field should be equal to $0 \ \mathrm{W \, m^{-2}}$. A non-null value is equivalent to applying a constant forcing to the model. It appears that our set of experiments exhibits this non-desired behaviour, coming from the fact that the whole system was not exactly at equilibrium after the time period. In order to remove that parameter dependant bias, a constant value is added to each such that the resulting average forcing is the same for each experiment, with a value of $-0.486 \ \mathrm{W \, m^{-2}}$. Figure A1 illustrates the average of the annual AHC across the set of 15 experiments.

A1 Interpolation scheme

Each of our 81 HadSM3 experiments should have a correct AHC field prescribed. However, the few datasets available made the use of a GPR impractical. Therefore, we opted for a more general Inverse Distance Weighting (IDW) interpolation scheme.

We designate $\boldsymbol{x}_i = [\tilde{e}_i \sin \varpi_i, \tilde{e}_i \cos \varpi_i, \tilde{\varepsilon}_i]^\top \in [-1, 1]^3$ as the vector that encapsulates the orbital parameters. These parameters are linearly rescaled to ensure that each one falls within the same range.

Subsequently, an interpolated value of the AHC can be computed as the weighted sum of the entire set. In this context, each weight is determined by the inverse square distance between the new point and the data, indicating that the weight is inversely proportional to the square of the distance.

$$\mathbf{Y}(\boldsymbol{x}) = \begin{cases} \mathbf{Y}_i & \text{if} \quad \boldsymbol{x} = \boldsymbol{x}_i \\ \frac{\sum_{i=1}^{N}(\boldsymbol{x}-\boldsymbol{x}_i)^{-2}\mathbf{Y}_i}{\sum_{k=1}^{N}(\boldsymbol{x}-\boldsymbol{x}_k)^{-2}} & \text{otherwise} \end{cases} \tag{A1}$$
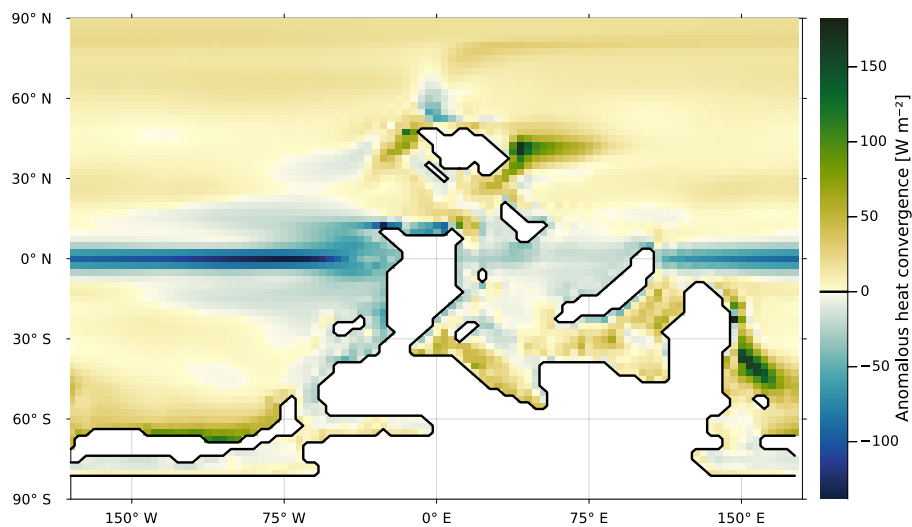
Figure A1. Ensemble mean of the annual AHC, expressed in Wm^{-2}.
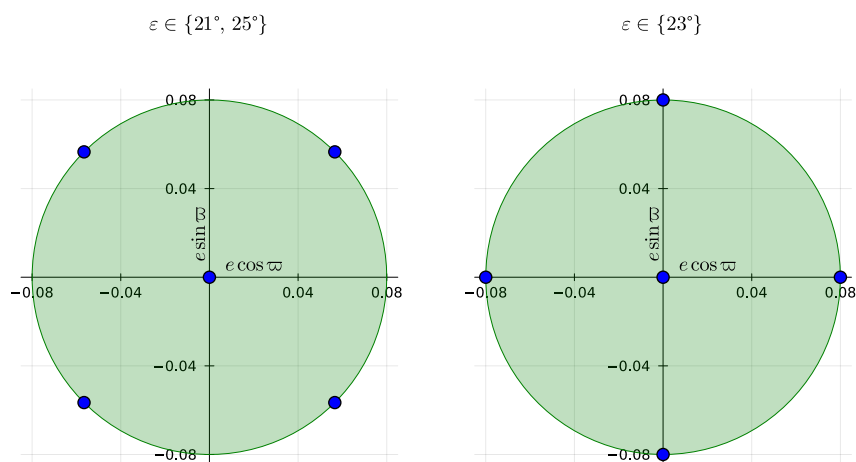

Figure A2. Slices of the cylinder constituting our HadCM3 experimental plan. The green area illustrates the possible value used during the interpolation process.

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