

## RESEARCH ARTICLE

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# Bayesian functional emulation of CO<sub>2</sub> emissions on future climate change scenarios

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## Abstract

We propose a statistical emulator for a climate-economy deterministic integrated assessment model ensemble, based on a functional regression framework. Inference on the unknown parameters is carried out through a mixed effects hierarchical model using a fully Bayesian framework with a prior distribution on the vector of all parameters. We also suggest an autoregressive parameterization of the covariance matrix of the error, with matching marginal prior. In this way, we allow for a functional framework for the discretized output of the simulators that allows their time continuous evaluation.

## KEYWORDS

Bayesian statistics, functional regression, hierarchical modeling, mixed effects model, uncertainty quantification

## 1 | INTRODUCTION

Climate change is, by far, the biggest and most life-threatening challenge of the present time. Its consequences have the potential to change our society and to threaten the very existence of humankind on this planet. With its intricate nature, climate change is a multidisciplinary issue that encompasses a variety of fields such as physics, chemistry, engineering, economics and sociology from the natural, human, and social sciences. Given the complexity of the interaction between different systems that constitute our society and climate, in recent years, the scientific community has employed several integrated assessment models (IAMs) to analyze the effects of climate change. These complex models are deterministic computer simulations, hence they consistently produce the same results with each run, given the same inputs. IAMs are generally designed to simulate the multidisciplinary aspect of a problem by combining various inputs from different fields. Large scale computer simulations of this nature are widely utilized in modern scientific research to study physical phenomena that are either too costly or impossible to replicate directly (Fan et al., 2009; Textor et al., 2005). These simulations are used to quantify how uncertainty in the input variables affects the output and how much uncertainty is introduced through the modeling process. The research goal is often to determine the distribution of one or multiple outputs of interest.

Generating the same outputs with several IAMs (namely, creating a model ensemble) allows to quantify one source of uncertainty. In this context we also deal with uncertainty due to the IAMs input. The scientific community has adopted a scenario approach to address the uncertainty in climate change modeling, utilizing Shared Socio-economic Pathways (SSPs) as inputs for IAMs. Scenario-based projections of future greenhouse gas emissions are crucial for estimating climate impacts and determining the necessary mitigation efforts for climate stabilization. The adoption of SSPs

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as part of a new framework enables a more integrated analysis of future climate impacts, vulnerabilities, adaptation, and mitigation within the climate change research community. See Moss et al. (2010), Van Vuuren et al. (2014), O'Neill et al. (2014), and Kriegler et al. (2014) for more details on the scenario process and SSPs framework. Note that an SSP consists in the discretization of a continuous plane of mitigation, that is, reducing the modification in climate induced by human activity, and adaptation to climate change (Riahi et al., 2017) as in Figure 1. Five scenarios have been identified within the SSPs framework. Among these, three align with the main diagonal, depicting futures where the challenges for climate change adaptation and mitigation are either low (SSP1), intermediate (SSP2), or high (SSP3). Additionally, two asymmetric scenarios exist that fall outside of the main diagonal. Specifically, SSP4 presents high challenges for adaptation with low challenges for mitigation, while the reverse is true for SSP5. Craigmile and Guttorp (2022) consider a similar context, analyzing multiple time series of temperatures with shared inputs, in order to produce a timely estimate of the annual global mean temperature. Global mean temperature is a commonly used diagnostic of climate change. Craigmile and Guttorp (2022) successfully model the discrepancies among various global temperature series by combining estimates and identifying potential sources of variation. They have been able to prove that the global temperature has increased  $1.2^{\circ}\text{C}$  with a standard error of  $0.03^{\circ}\text{C}$  over the 1880–1900 average and that the probability that 2020 was the warmest year on record is 0.44.

The output of a simulator, such as an IAM, will always be imperfect due to the limitations of computer predictions of real phenomena. Certain aspects of carbon dioxide ( $\text{CO}_2$ ) simulation scenarios, such as the infinite possible starting values and running times, cannot be known with certainty. Additionally, it could be unfeasible to run the model for every input parameter combination, or it could be expensive. As stated in O'Hagan (2006), statistical analysis should account for the biases in the model or input representation. The goal is to have a single, fast statistical emulator that can capture all variability induced by the simulators (Kennedy & O'Hagan, 2001; Santner et al., 2003). Specifically, a statistical emulator is a statistical model that represents data generated by various IAMs. This approach addresses the challenge of large computer simulations by treating IAMs as black boxes and modeling the uncertainty in a non-intrusive manner. An effective emulator provides accurate approximations of the computer code output for a wide range of input values and quantifies the uncertainty accurately (see Francom et al., 2018). The biggest advantages of this approach are the ability to evaluate outputs with different inputs, even after emulating the process (Busby, 2009) and to provide error intervals for unseen inputs, fulfilling the basic requirements for uncertainty quantification.

In simpler terms, an emulator is a stochastic representation of a computer model that predicts its output and reports the measure of uncertainty for that prediction. Francom et al. (2019) present a recent study on Bayesian emulation, proposing an innovative method based on adaptive splines for modeling simulations of the dispersal of radioactive particles in the atmosphere. However, a popular approach is based on Gaussian process-based emulation methods. For example, Bayarri et al. (2007) develop a model that effectively handles highly irregular functional data and incorporates uncertainty in the inputs for the analysis of dynamic stress in engineering systems, and Higdon et al. (2008) assume GP models to simulate output from the simulator at untested input configurations and incorporated them into a comprehensive framework to facilitate parameter estimation and prediction for characterizing material properties, a particularly useful approach when dealing with highly multivariate field data and simulator output. In the context of emulating time series output

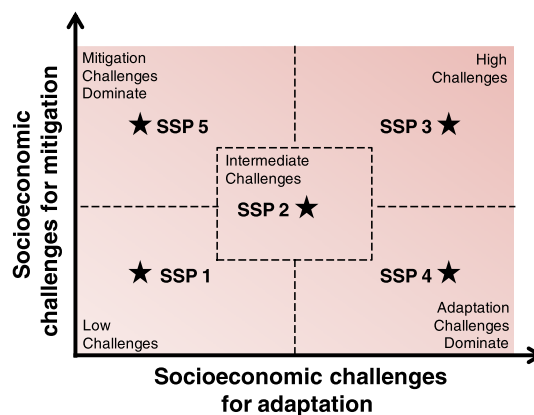


FIGURE 1 SSPs plane on adaptation and mitigation, based on Figure 1 from O'Neill et al. (2014).

from computer simulations, Liu and West (2004) effectively combine Bayesian multivariate dynamic linear models with Gaussian process modeling, as demonstrated with data from a hydrological simulation model. Similarly, Williamson and Blaker (2014) develop Bayesian dynamic linear model Gaussian processes for emulating time series output from computer models that may exhibit chaotic behavior, while retaining some underlying structure.

Functional regression, a technique used in functional data analysis (FDA, Ramsay et al., 2005), can be employed to design emulators for continuous phenomena such as CO<sub>2</sub> emissions. The functional framework is particularly suitable for discrete simulation outputs of continuous phenomena, as it allows for modeling the underlying functional relationship between predictor and response variables. By leveraging functional regression, emulators can be developed to accurately describe and approximate the continuous nature of the phenomenon under consideration, enabling effective prediction and simulation of the target process. Functional regression variants include: scalar-on-function, function-on-function, and function-on-scalar. Scalar-on-function regression models a scalar response variable as a function of one or more functional predictor variables, while function-on-function regression involves modeling a functional response variable as a function of functional predictor variables. Instead, function-on-scalar regression (FOSR) models a functional response variable as a function of scalar predictor variables. Since, as shown in Section 2, our input data are scalars, to statistically emulate these deterministic simulators, we have adopted the FOSR framework. This approach extends the traditional linear regression by incorporating functional responses and functional regression coefficients, which adds to the difficulty of estimation, inference, and interpretation. See, for instance, Nie et al. (2023) for an example of such difficulty, in a scalar-on-function perspective. In particular, they predict the total daily bike rentals by utilizing hourly temperature data, successfully identifying the time regions where the functional predictor effectively correlates with the response. FOSR has a wide range of interesting applications, including blood pressure profiles during pregnancy (Montagna et al., 2012), longitudinal genome-wide association studies (Barber et al., 2017; Fan & Reimherr, 2017), and analyzing actigraphy data to investigate the connection between physical activity and sleep questionnaire responses (Kowal & Bourgeois, 2020). Despite its similarities with multivariate regression, FOSR presents additional modeling challenges. The dependence within functional data must be modeled with care, which may require complex or additional assumptions about the covariance structure. This affects the model's flexibility, computational complexity, and scalability.

In this study, the output of the IAMs include projections of several variables, with a focus on CO<sub>2</sub> emissions, as it is the most widely studied variable affecting the climate. The data consists of  $23 \times 5$  CO<sub>2</sub> global emission profiles, expressed in GtCO<sub>2</sub>, which are time-dependent and discretized with a 10-year frequency for computational efficiency. The high cost and demanding nature of these massive simulations prompted the decision to use a lower frequency in the output, as a higher frequency would increase the computational cost and the time required to run the model. The CO<sub>2</sub> emissions were calculated as the output of five different IAMs, using the same combinations of SSP variables such as gross domestic product and fossil fuel availability. The number of total combinations is 23. The data we consider are the same as in Marangoni et al. (2017), and we use only the SSPs scenarios aligned with the main diagonal as depicted in Figure 1. As described in Riahi et al. (2017), this figure shows a continuous plane divided in 5 parts, representing five different future challenges. Treating such plane as continuous allows us to represent a diverse and continuous range of future socioeconomic trajectories, providing a more comprehensive and flexible tool for scenario analysis and policy assessment.

We adopt a Bayesian approach to analyze CO<sub>2</sub> emission profiles. Our analysis is based on a Bayesian multilevel hierarchical model, which is a popular method for longitudinal data analysis (Daniels & Pourahmadi, 2002; Shen & Liu, 2020). This model allows to estimate the scores of the basis expansions of the regression coefficients, a technique from FDA useful to represent a function through certain basis. Our modeling choice is similar to the one proposed by Goldsmith and Kitago (2016), which focuses on the functional representation of the trajectories of the arm of patients affected by stroke. However, we introduce a different form of the parametric covariance structure for the within-function correlation, which ease the computations and allow for a predictive inference. The Bayesian approach offers several benefits, including the ability to incorporate multiple sources of information and uncertainty, and a greater flexibility to build complex models. The hierarchical modeling framework is well-suited to our application, as it allows us to describe different types of grouped data, such as multilevel data from multiple subjects. In our case, the group is the combination of SSPs input for the IAMs, as we are interested in evaluating how simulation inputs affect outputs. Our Bayesian model uses a prior distribution for all group-specific parameters that borrows information from the largest groups to estimate parameters from the smallest ones and allows to describe the new uncertainty of the parameters after seeing the data.

The original contributions of this work includes the proposal of a Bayesian model for simulator data, specifically designing the likelihood and the prior for the data at hand. Posterior inference of the simulator data can be interpreted

from a probabilistic perspective, providing a measure of how much each SSP contributes to the IAMs output. As a by-product of our approach, we also obtain an estimate of the variability of the SSP combinations induced by different IAMs, with a credible interval provided for a new IAM simulator. We also obtain evaluation of emissions at any time beyond the simulation output. MCMC simulations for computing posterior inference have been obtained using *Stan* (Stan Development Team, 2023) and *R* (R Core Team, 2022) codes.

The outline of this manuscript is as follows. Section 2 describes the data. In Section 3, we present the Bayesian model that we have fitted to the data. In Section 4, we demonstrate the application of our approach to the data and present posterior inference and findings. The article concludes with a discussion and potential future developments in Section 5. Supplementary materials contain additional information on the selection of hyper-parameters, sensitivity analysis, and supplementary images that have been omitted from the main manuscript.

## 2 | DATA

Data are those from the study by Marangoni et al. (2017). Additional information and details on SSPs can be found on the International Institute for Applied System Analysis (IIASA) website. We analyze the output of 5 IAMs. Each IAM produces 23 distinct time series, each corresponding to 23 different inputs, with a 10-year interval, for global CO<sub>2</sub> emissions (expressed in gigatons of carbon dioxide, i.e., GtCO<sub>2</sub>).

Each input to an IAM is a combination of future projection scenarios for the following SSP variables: population (**POP**), gross domestic product per capita (**GDPPC**), energy intensity improvements (**END**), fossil fuel availability (**FF**), and low-carbon energy technology development (**LC**). In each of the 23 combinations, the scenarios for the variables belong to one of three levels: SSP1, SSP2, or SSP3. The SSPs variables are not treated as functions but rather as scalars, as we adopt the same experimental strategy as Marangoni et al. (2017). More precisely, we map a given pathway to a specific level of the corresponding SSP variable. The SSPs plane is assumed to be continuous (as shown in Figure 1). The two main drivers on which they are built (challenges to mitigation and challenges to adaptation) must not be perceived as discrete factors, but rather as continuous ones, representing a continuity of levels for both challenges to adaptation and challenges to mitigation.

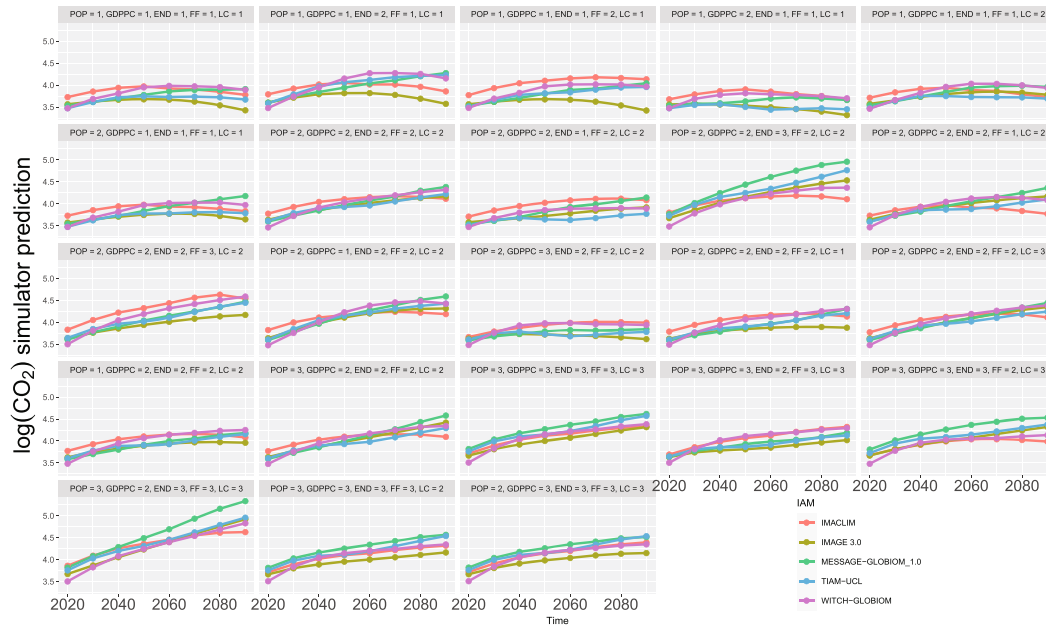
While SSPs are often presented as discrete levels (e.g., SSP1, SSP2, SSP3, etc.) for practical purposes and ease of communication, they are designed to be interpreted as points along a continuous spectrum, with the understanding that values can exist between the defined SSP levels. This is motivated by the fact that the SSP framework provides a range of plausible future pathways that span a continuum of socioeconomic conditions, allowing for a more nuanced representation of future uncertainties. For example, if **GDPPC** is assigned a value of 1 and all other variables are assigned a value of 2, this combination indicates that **GDPPC** follows the SSP1 pathway and all others follow the SSP2 pathway. The choice to treat the variables as continuous rather than discrete is also motivated by the ability to make predictions for scenarios that lie halfway between two levels (e.g., **GDPPC** = 2.5).

Assuming a continuous nature for SSPs does imply a constant difference or increment between SSP levels, which might not always reflect the true dynamics of socioeconomic development. The differences between SSP levels may not be uniform, and the magnitude of change in variables such as population, economy, technology, and energy use may vary non-linearly between different SSP levels. However, our approach provides a framework to explore a wider range of potential future scenarios that may not fit neatly into discrete categories, accommodating gradual transitions and intermediate pathways. Moreover, it can help fill data gaps or generate plausible scenarios for SSPs combinations not used as input, enabling a more comprehensive and consistent analysis. It can also enhance comparability between different scenarios or models, allowing for a common framework to evaluate the implications of different SSP levels and facilitating meaningful comparisons of outcomes and impacts across different SSP-based scenarios.

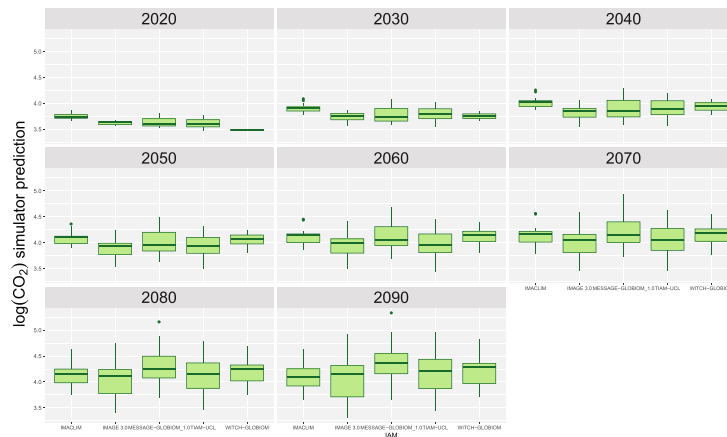
The data we consider have the following structure:

$$\mathbf{y}_{ij} = [y_{ij}(t_1), \dots, y_{ij}(t_D)] \quad \mathbf{w}_i = [1, w_{i1}, \dots, w_{ip}]^T \quad j = 1, \dots, J, \quad i = 1, \dots, I,$$

where  $J = 5$  and  $I = 23$  are, respectively, the number of IAMs and SSPs combinations,  $\{t_1, \dots, t_D\} = \{2020, \dots, 2090\}$  with  $D = 8$ . Here  $\mathbf{w}_i$  represent the  $i$ th combination of SSP variables, including an intercept term, with  $p = 5$ ;  $\mathbf{y}_{ij}$  is the CO<sub>2</sub> profile emission, in logarithmic scale, produced by the  $i$ th SSP combination within the  $j$ th IAM. The total number of observations is  $N = I \times J$ . Figure 1 in the Supplementary materials contains five panels, each representing a different IAM and displaying 23 different emission profiles. These plots illustrate the diverse projection ranges across time produced by



**FIGURE 2** CO<sub>2</sub> emissions profiles in logarithmic scale grouped by SSP combination; each panel displays the five output from the same SSP combination.



**FIGURE 3** Boxplots of CO<sub>2</sub> emissions (in the log scale) by IAMs for each decade. The range of the y-axis is the same.

different IAMs, which are primarily due to variations in their assumptions and implementation. Our modeling approach will aim to model these differences. Figure 2 presents, for each of the 23 combinations of SSPs variables, the five curves corresponding to different IAMs. It is evident within each panel that the IAM curves are correlated. As a result, we will model this dependence through the use of random effects. Finally, Figure 3 displays box-plots comparing the emissions per decade produced by the five IAMs. It is important to note that the box-plots for each decade vary across the IAMs.

### 3 | BAYESIAN FUNCTIONAL MODEL

In Section 2, we have introduced notation for our data, that is,  $y_{ij}(t_d)$  as the logarithm of the CO<sub>2</sub> emission at time  $t_d$  produced by the  $j$ th IAM given the  $i$ th SSPs combination  $\mathbf{w}_i = [1, w_{i1}, \dots, w_{ip}]^T$  as input, with  $p = 5$ . We assume, for any fixed  $t$ , for each SSPs combination  $i = 1, \dots, I$  and for each IAM  $j = 1, \dots, J$ :

$$y_{ij}(t) = \mathbf{w}_i^T \boldsymbol{\beta}(t) + c_i(t) + \epsilon_{ij}(t), \quad (1)$$

where  $\epsilon_{ij}(t)$  is a Gaussian random error with 0 mean and variance that we specify below, and  $\boldsymbol{\beta}(t) = [\beta_0(t), \dots, \beta_p(t)]$  is the corresponding regression parameter at time  $t$ . Here  $c_i(t)$  is the  $i$ th SSP combination specific random effect coefficient function, that models the internal variability of the combination and induce correlation between observations with the same SSPs combination as input.

### 3.1 | Functional representation

We rely on functional representation of the IAMs output since we assume the CO<sub>2</sub> emission simulations as a (smooth) continuous phenomenon in time, and whose temporal downscaling is of great interest. Here, by temporal downscaling, we mean the ability to assess and evaluate the output of the IAM for any time instant, and not only for those at which the IAMs output were produced. The functional approach will be useful to approach the problem.

Hence we consider a FOSR model for the response curves  $\{y_{ij}(t)\}$ , expanding all the regression parameters  $\{\beta_k(t), k = 0, 1, \dots, p\}$  and random effects  $\{c_i(t), i = 1, \dots, I\}$  via a truncated B-spline basis expansion with  $K$  components (for more details, see Ramsay et al., 2005). More explicitly, we assume that

$$\beta_k(t) = \sum_{l=1}^K b_{lk} \theta_l(t) \quad k = 0, 1, \dots, p, \quad (2)$$

where  $\{\theta_l(t), l = 1, \dots, K\}$  is the B-spline basis and  $\{b_{lk}, l = 1, \dots, K\}$  are the unknown scores of the functional parameters  $\beta_k(t)$  expansion. Similarly we assume

$$c_i(t) = \sum_{l=1}^K d_{li} \theta_l(t) \quad i = 1, \dots, I, \quad (3)$$

where  $\{d_{li}, l = 1, \dots, K\}$  are the unknown scores of the functional random effect  $c_i(t)$  expansion. Equation (1) becomes, in a vectorized form, the following

$$\mathbf{y}_{ij} = \mathbf{w}_i^T \boldsymbol{\beta} + \mathbf{z}_i^T \mathbf{c} + \epsilon_{ij}, \quad \epsilon_{ij} | \boldsymbol{\Sigma} \stackrel{iid}{\sim} \mathcal{N}_D(\mathbf{0}, \boldsymbol{\Sigma}), \quad (4)$$

where  $\boldsymbol{\beta} = [\beta_k(t_d)]_{k,d}$  is the unknown  $(p+1) \times D$  matrix whose rows are the regression coefficients functions evaluated at the time grid,  $\mathbf{z}_i$  is the  $I \times 1$  vector indicating the SSP scenario combination with all 0 elements but a 1 in the  $i$ th position,  $\mathbf{c} = [c_i(t_d)]_{i,d}$  is the unknown  $I \times D$  matrix of subject random effects and  $\epsilon_{ij} = [\epsilon_{ij}(t_1), \dots, \epsilon_{ij}(t_D)]^T$  is the  $D$ -dimensional error vector with  $\mathbf{0}$  mean and covariance matrix  $\boldsymbol{\Sigma}$ .

Expanding  $\{\beta_k(t)\}$  and  $\{c_i(t)\}$  as in (2) and (3) respectively, the matrices  $\boldsymbol{\beta}$  and  $\mathbf{c}$  in (4) assume the following form:

$$\boldsymbol{\beta} = [\boldsymbol{\Theta} \mathbf{B}_W]^T \quad \mathbf{c} = [\boldsymbol{\Theta} \mathbf{B}_Z]^T \quad (5)$$

with  $\boldsymbol{\Theta} = [\theta_l(t_d)]_{d,l}$  being the known  $D \times K$  cubic B-splines evaluation matrix. Here  $\mathbf{B}_W = [b_{l,k}]_{l,k}$  is the  $K \times (p+1)$  matrix whose columns contain the fixed effects basis scores vector to be estimated and  $\mathbf{B}_Z = [d_{l,i}]_{l,i}$  is the  $K \times I$  matrix whose columns are the random effects basis scores vector to be estimated as well.

### 3.2 | Hierarchical model

With the basis expansion described in (5), model (4) is equivalent to the following:

$$\mathbf{y}_{ij} = \mathbf{w}_i^T \mathbf{B}_W^T \boldsymbol{\Theta}^T + \mathbf{z}_i^T \mathbf{B}_Z^T \boldsymbol{\Theta}^T + \epsilon_{ij} \quad \epsilon_{ij} \stackrel{iid}{\sim} \mathcal{N}_D(\mathbf{0}, \boldsymbol{\Sigma})$$

for  $i = 1, \dots, I$  and  $j = 1, \dots, J$ . For a more efficient MCMC sampling performance, the model is hierarchically centered as in Gelfand et al. (1995), that is, for  $i = 1, \dots, I$  and  $j = 1, \dots, J$ :

$$\mathbf{y}_{ij} = \mathbf{z}_i^T \mathbf{B}_Z^T \boldsymbol{\Theta}^T + \epsilon_{ij} \quad \text{with} \quad \epsilon_{ij} \stackrel{iid}{\sim} \mathcal{N}_D(\mathbf{0}, \boldsymbol{\Sigma}) \quad (6)$$

with centered priors

$$\begin{aligned} \mathbf{B}_{Z,i} | \mathbf{B}_W, \sigma_Z^2 &\stackrel{ind}{\sim} \mathcal{N}_K(\mathbf{B}_W \mathbf{w}_i, \sigma_Z^2 \mathbf{P}^{-1}) \quad \sigma_Z^2 \sim IG(a_Z, b_Z) \quad i = 1, \dots, I \\ \mathbf{B}_{W,k} | \sigma_{W,k}^2 &\stackrel{ind}{\sim} \mathcal{N}_K(\mathbf{0}, \sigma_{W,k}^2 \mathbf{P}^{-1}) \quad \sigma_{W,k}^2 \stackrel{ind}{\sim} IG(a_{W,k}, b_{W,k}) \quad k = 0, 1, \dots, p, \end{aligned} \quad (7)$$

where  $a_Z, b_Z, a_{W,k}$ , and  $b_{W,k}$  are fixed hyperparameters. Model (6) and (7) is very similar to the model in Goldsmith and Kitago (2016), but as it will be clear in a while, we introduce a different covariance structure on the error. In (7) we assume the  $K \times K$  matrix  $\mathbf{P} = \alpha \mathbf{P}_0 + (1 - \alpha) \mathbf{P}_2$  as a penalization matrix which is constructed as a weighted sum of two different matrices concerning shrinkage (i.e.,  $\mathbf{P}_0$ ) and smoothness (i.e.,  $\mathbf{P}_2$ ). Further details on the construction of the components of  $\mathbf{P}$  are present in Eilers and Marx (1996).

We assume an autoregressive configuration for the covariance matrix  $\boldsymbol{\Sigma}$  of the errors

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma^2 & \sigma^2 \rho & \dots & \dots & \sigma^2 \rho^{D-1} \\ \sigma^2 \rho & \ddots & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \sigma^2 \rho \\ \sigma^2 \rho^{D-1} & \dots & \dots & \sigma^2 \rho & \sigma^2 \end{bmatrix}. \quad (8)$$

In a first version of this work (Aiello, 2020) we have assumed  $\boldsymbol{\Sigma}$  as a full matrix and given it an IW prior distribution. However, posterior computations were much heavier and the associated inference gave evidence to the autoregressive assumption (8). We complete the prior specification assuming prior independence among  $\sigma^2$ ,  $\psi$ , and  $\rho$ , and:

$$\sigma^2 \sim IG\left(\frac{\nu}{2}, \frac{\nu}{2} \psi\right) \quad \psi \sim \Gamma\left(\frac{\nu_0}{2}, \frac{\nu_0}{2} \frac{1}{\psi_0}\right) \quad \rho \sim \mathcal{N}(0, 1), \quad (9)$$

where  $\nu$ ,  $\nu_0$ , and  $\psi_0$  are fixed hyperparameters. Observe that (8) is a first order autoregressive, that is,  $AR(1)$ , covariance structure over time. The correlation between two successive decades is assumed homogeneous over time in (8) and denoted by  $\rho$ . This parameterization for  $\boldsymbol{\Sigma}$  will result particularly convenient for computing predictions at times not included in the IAMs output. Through model (6)–(9) we reduced the infinite dimensional problem to a finite dimensional one.

## 4 | APPLICATION

In this section, we assume model (6)–(9) for the data from the IAM model ensemble discussed in Section 2. Each SSP combination, represented by the vector  $\mathbf{w}_i$ , is a 6-dimensional input including an intercept term, with multiple curves associated with it for each IAM. We fix the number of B-spline basis to  $K = 8$ , and the adjusting parameter between shrinkage and smoothness to  $\alpha = 0.01$  in  $\mathbf{P} = \alpha \mathbf{P}_0 + (1 - \alpha) \mathbf{P}_2$  in order to give more weight to smoothness. We fixed  $a_{W,k} = 4$  for all  $k = 0, \dots, p$ ,  $\mathbf{b}_W = [0.51, 0.0002, 0.002, 0.001, 0.0005, 0.0001]^T$ ,  $a_Z = 92$ ,  $b_Z = 0.0038$  (see (7) for definition of these hyperparameters),  $\nu = 7$ ,  $\nu_0 = 2$ , and  $\psi_0 = 0.047$  (see (9)). See the Supplementary materials for details on this choice.

Posterior inference for this study was obtained using Stan and rstan package (Hoffman & Gelman, 2014; Stan Development Team, 2023). Stan is an open-source, general-purpose programming language for Bayesian analysis, and rstan serves as an interface with R (R Core Team, 2022). The codes used for this study can be found in the Supplementary materials. To ensure robust results, four chains were run in parallel using Stan, with each chain consisting of 20,000 iterations. The first 15,000 iterations were discarded, resulting in a final sample size of  $R = 20,000$ . Further information on

the sensitivity analysis associated with hyperparameters can be found in the Supplementary materials. To visualize chain diagnostics, traceplots and autocorrelation plots of the expansion scores of the **POP** regression coefficient are provided in Figures 3 and 4 of the Supplementary materials.

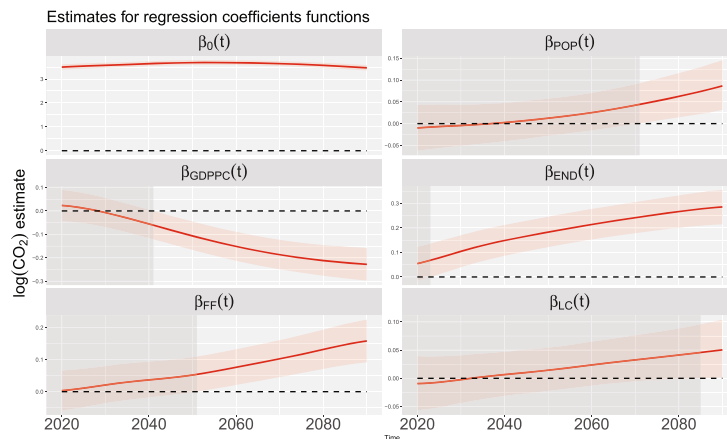
#### 4.1 | Regression coefficient functions

We report here the estimate of the functional regression parameters  $\{\beta_k(t), k = 0, 1, \dots, p\}$ . More precisely, having access to the simulated posterior values of  $\mathbf{B}_W = [b_{l,k}]_{l,k}$ , the estimates of the regression coefficient functions can be computed as:

$$\mathbb{E} [\beta_k(t)|data] = \frac{1}{R} \sum_{r=1}^R \boldsymbol{\Theta}(t) \mathbf{B}_{W,k}^{(r)} \quad k = 0, 1, \dots, p, \quad (10)$$

where  $R$  is the final sample size,  $\boldsymbol{\Theta}(t) = [\theta_l(t)]_l$  is the vector containing the basis functions and  $\mathbf{B}_{W,k}^{(r)}$  is the current MCMC value of the column vector  $\mathbf{B}_{W,k}$  in the MCMC (see (5)). Figure 4 presents the estimated regression coefficient functions, computed as in (10), over a detailed grid of values of  $t$  in the range [2020, 2090]. The plots display the simultaneous 95% posterior credible bands, as well as the time points where the 95% credibility interval does include zero, indicated by gray shading. This provides a useful tool to evaluate the significance of the regression coefficients as they vary over time. The time interval in which zero is not included in the credibility band indicates that the variable is significantly different from zero.

The functional data approach used in model (1) enables estimation, visualization, and assessment of the regression coefficient functions, which is important for determining the time intervals where effects are strong and those where they are null or negligible. The variation in each  $\beta_k(t)$  over time is another key aspect that will be discussed further. The posterior credible bands of the coefficients corresponding to **GDPPC** and **END** exclude zero around 2040 and 2020, respectively. This provides evidence to consider them as the main driving fixed effects in the IAMs simulations. Additionally, they are the coefficients that deviate the most from zero, indicating that their impact is substantial. The regression coefficient function for **GDPPC** has a negative effect, while the other coefficients have a positive effect. This negative effect can be explained by the scenario SSP1, which assumes a world that is wealthier than in SSP3. A wealthier population is expected to consume and pollute more than a poorer one. Covariates **FF** and **POP** become significant after 2050 and 2070, respectively. Although their coefficients are not as large as those for **GDPPC** and **END**, they can also be considered significant. Variable **LC** does not appear to be significant. For an alternative assessment of the significance of the coefficients, please refer to Figure 5 of the Supplementary materials.



**FIGURE 4** Estimates of the regression coefficient  $\beta_k(t)$ , obtained via B-spline basis expansion. The estimate is obtained as the posterior mean (10) and denoted as solid red line.

## 4.2 | Emission curve estimation

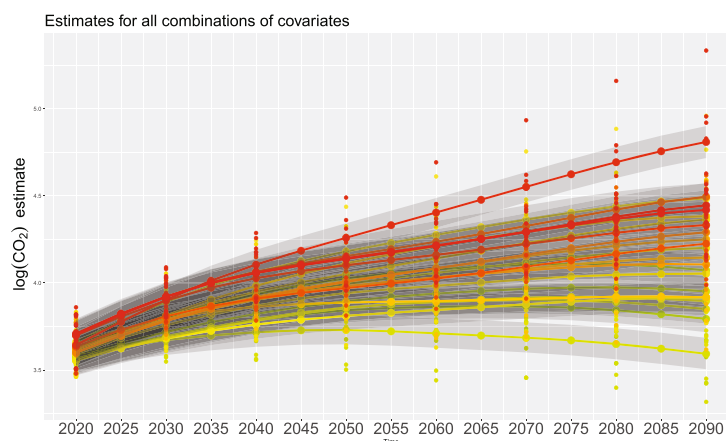
The benefit of estimating the expansion score matrix  $\mathbf{B}_Z$  alongside other parameters is that it enables us to calculate the parameters representing the conditional expectation of  $y_{ij}(t)$  in (6). This is done by computing the posterior mean of the functional random effects parameters  $c_i(t)$  as outlined in (1) through representation (6). Specifically we compute  $\mathbb{E}[c_i(t)|data]$  for  $i = 1, \dots, I$  through the MCMC output, similarly as in (10) starting from posterior draws of  $\mathbf{B}_Z$ . The posterior estimate represents the Bayesian estimates of the logarithm of CO<sub>2</sub> emission at any time point  $t$  in the interval [2020, 2090]. Figure 5 shows the posterior mean of  $c_i(t)$  along with 95% credibility intervals simultaneously.

To better understand the estimates shown in Figure 5, we have plotted, in Figure 6, the mean and 95% simultaneous credible bands over time of the posterior distribution of  $c_i(t)$ , for the combinations of SSP that have the same value in each SSP variable. These combinations include  $\mathbf{w}_{i_1} = (1, 1, 1, 1, 1, 1)^T$ ,  $\mathbf{w}_{i_2} = (1, 2, 2, 2, 2, 2)^T$ , and  $\mathbf{w}_{i_3} = (1, 3, 3, 3, 3, 3)^T$ . The min–max data range is also depicted in the figure, indicated by the gray shading. Compared to the standard approach for uncertainty quantification in computer simulators, which is commonly followed for IAMs, our approach provides a more probabilistic measure of uncertainty. This is achieved by computing the full posterior distribution of the IAMs output mean, which is specific of the input given by the SSPs. Currently, the uncertainty quantification of IAMs is carried out through an empirical evaluation of the output from different simulators. Our method has several advantages in terms of interpreting the estimates, as it allows for a true probabilistic interpretation of the results. Figure 6 shows that the commonly used empirical approach only considers deterministic ranges (represented by the gray bands) while our approach uses the proper posterior distribution for emissions at unseen data points, enabled by a functional framework. This is a new feature in IAMs, which typically rely on empirical ranges to quantify uncertainty. Our method not only incorporates uncertainty in the multi-IAM framework but also provides probabilistic meaning to the parameter estimates, a unique aspect in such simulations.

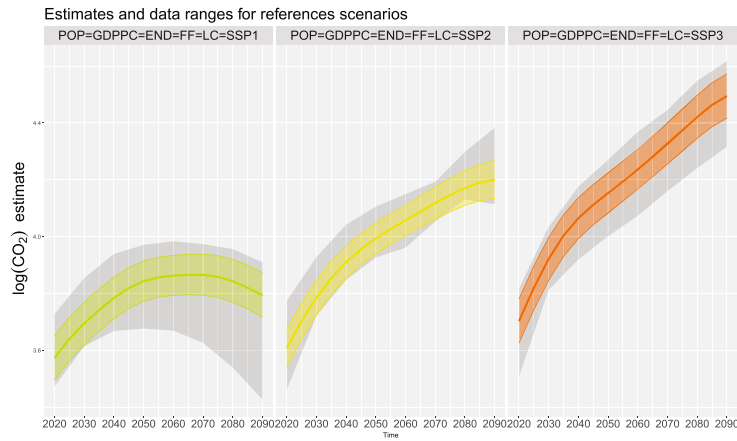
The posterior predictive MSE under our model shows only minimal deviation from the MSE calculated through empirical estimates, as in Chapter 13 of Ramsay et al. (2005). Our model MSE stands at 0.016, while the frequentist estimate is 0.014, with the latter being slightly more optimal. However, we prefer our model due to the numerous benefits it presents as a Bayesian approach, which have been discussed throughout the article. For reference, a comparison of the three estimates between the two approaches can be found in Figure 2 of the Supplementary materials.

## 4.3 | Temporal kriging

To perform predictive temporal downscaling, we have chosen a kriging approach specifically designed to meet our needs. Our objective is to predict the emission values for each IAM and SSPs combination at mid-decade intervals (e.g., 2025, ..., 2085). To accomplish this, we have implemented an augmented data approach where the response variables considered are:



**FIGURE 5** Posterior mean of  $c_i(t)$  corresponding to the 23 combination of SSPs in the study with 95% credibility bands associated; points are the observed outputs given by the IAMs.



**FIGURE 6** Posterior mean of the  $c_i(t)$ 's, with associated 95% credible bands, under different values of  $\mathbf{w}_i$ . The gray bands represent the convex hull of the empirical trajectories of  $\log(CO_2(t))$ .

$$\tilde{\mathbf{y}}_{ij} = [y_{ij}(t_1), \dots, y_{ij}(t_{\tilde{D}})],$$

where, in this case,  $t_1 = 2020, t_2 = 2025, t_3 = 2030, t_4 = 2035, \dots, t_{\tilde{D}} = 2090$  with  $\tilde{D} = 15$ . The model for these augmented data is exactly the same as in (6) where matrices  $\tilde{\Theta}$  and  $\tilde{\Sigma}$  are defined as  $\Theta$  and  $\Sigma$ , respectively, with the proper changes of dimensions, based on a Gaussian process. Specifically, we assume:

$$\tilde{\mathbf{y}}_{ij} | \mathbf{B}_Z, \tilde{\Sigma} \stackrel{ind}{\sim} \mathcal{N}_{\tilde{D}}(\mathbf{z}_i^T \mathbf{B}_Z^T \tilde{\Theta}^T, \tilde{\Sigma}).$$

We differentiate between the emissions that have been observed at full decades and those that have not been observed, that is, at mid-decades. In instances where observations are missing, the Bayesian approach enables us to treat them as random parameters. To achieve this, we incorporate them into the state space of the MCMC and generate simulations from their posterior predictive distribution. To be specific, we use MCMC samples drawn from the following distribution

$$\mathcal{L}(\mathbf{y}_{ij}^{\text{pred}} | \mathbf{y}^{\text{obs}}) = \int_{\Phi} \mathcal{L}(\mathbf{y}_{ij}^{\text{pred}}, d\phi | \mathbf{y}^{\text{obs}}) = \int_{\Phi} \mathcal{L}(\mathbf{y}_{ij}^{\text{pred}} | \phi, \mathbf{y}^{\text{obs}}) \pi(\phi | \mathbf{y}^{\text{obs}}) d\phi, \quad (11)$$

where  $\mathbf{y}_{ij}^{\text{pred}} = [y_{ij}(t_1), y_{ij}(t_3), \dots, y_{ij}(t_{\tilde{D}})]$ ,  $\mathbf{y}^{\text{obs}}$  contains all the observed data,  $\pi(\phi | \mathbf{y}^{\text{obs}})$  is the posterior of the vector of all the parameters of the model and  $\Phi$  is the space of all the model parameters. The distribution  $\mathcal{L}(\mathbf{y}_{ij}^{\text{pred}} | \phi, \mathbf{y}^{\text{obs}})$  can be computed from the joint distribution of  $\mathbf{y}^{\text{pred}}$  and  $\mathbf{y}^{\text{obs}}$ , which is a  $\tilde{D}$ -dim Gaussian density. From straight-forward computations we derive that

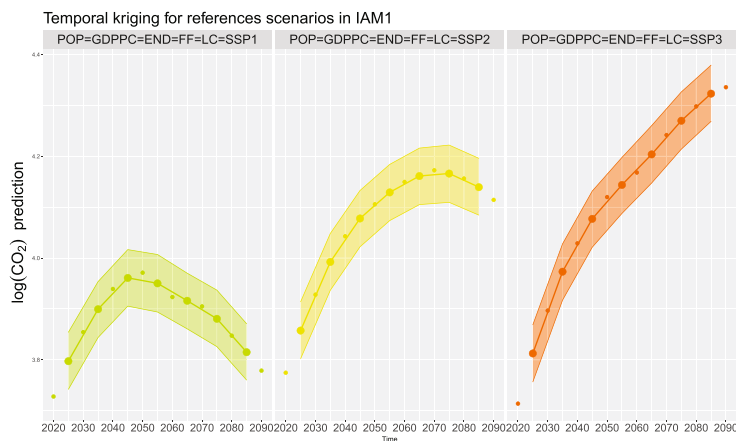
$$\mathbf{y}_{ij}^{\text{pred}} | \mathbf{B}_Z, \tilde{\Sigma}, \mathbf{y}_{ij}^{\text{obs}} \sim \mathcal{N}_{D_{\text{pred}}}(\bar{\mu}_{ij}, \bar{\Sigma}),$$

where

$$\begin{aligned} \bar{\mu}_{ij} &= \Theta_{\text{pred}} \mathbf{B}_Z \mathbf{z}_i + \Sigma_{\text{pred,obs}} \Sigma_{\text{obs,obs}}^{-1} (\mathbf{y}_{ij}^{\text{obs}} - \Theta_{\text{obs}} \mathbf{B}_Z \mathbf{z}_i) \\ \bar{\Sigma} &= \Sigma_{\text{pred,pred}} - \Sigma_{\text{pred,obs}} \Sigma_{\text{obs,obs}}^{-1} \Sigma_{\text{obs,pred}} \end{aligned}$$

with  $\Sigma_{\text{pred,pred}}$ ,  $\Sigma_{\text{obs,obs}}$ ,  $\Sigma_{\text{pred,obs}}$ , and  $\Sigma_{\text{obs,pred}}$  are the matrices relative to the predicted points covariance, to the observed points covariance, and to the covariance between observed and predicted points. Moreover,  $\Theta_{\text{pred}}$  is the submatrix of  $\tilde{\Theta}$  relative to the predicted points respectively.

Figure 7 displays the temporal kriging distribution for three curves of IAM 1, represented by large dots and shaded areas (the 95% credible band), as well as the smaller dots representing the observed data. The plot indicates that the observed data for IAM 1 lies within the 95% credible intervals of the estimated mean curves. This is significant because



**FIGURE 7** Temporal kriging for three reference scenarios of IAM 1.

computer models such as IAMs are very expensive to run and they are usually only run with a limited number of input points. Our procedure provides a useful tool for refining the temporal grid, reducing the computational burden of the simulator, and enabling researchers to draw conclusions based on multiple IAM outputs with decade-level frequencies.

## 5 | CONCLUSIONS

Climate change presents one of the most formidable obstacles humanity has ever encountered (Pachauri et al., 2014). To tackle this problem, reducing greenhouse gas emissions, particularly CO<sub>2</sub>, is crucial. Consequently, the scientific community has developed numerous computational models to simulate CO<sub>2</sub> emission patterns and other climatic variables over the next century. These models are complex and often expensive to run, limiting the number of runs and input parameters that can be tested. In recent years, statistical emulators have gained popularity as they imitate the behavior of the simulator by using a limited number of numerical outputs for data analysis.

We have proposed a Bayesian hierarchical model for simulation outputs with high flexibility and randomness in parameters. The Bayesian approach provides a tool for uncertainty quantification, a crucial aspect in this context. By computing the joint posterior distribution of all parameters, we can also estimate intervals based on the probabilistic model, thus quantifying the posterior probability of a parameter belonging to a specific interval. The continuous representation of IAM outputs is achieved through the functional framework, as we assume that IAM emissions are the smooth, simulated outputs of a phenomenon over time and space. The hierarchical structure of the model further allows for increased flexibility and improved estimation by incorporating group-specific parameters and sharing information between different groups. This is known as borrowing of information in Bayesian models.

We have chosen to use an AR(1) covariance structure for the likelihood, as this option reduces computational effort while enhancing the interpretability of the parameters. In a preliminary analysis, other models, such as time series models or multivariate regression, were also considered. However, the auto-regressive covariance structure is particularly suitable for temporal downscaling. The results of the posterior analysis indicate that the **GDPPC** and **END** are the most crucial factors in determining CO<sub>2</sub> emissions. This highlights the need for comprehensive and forward-thinking policies that address changes in the economic and energy sectors. Our findings also suggest that the availability of fossil fuels plays a significant role in predicting CO<sub>2</sub> emissions, although it is less impactful than other factors. However, the development of low carbon technologies does not seem to have much of an effect on simulated CO<sub>2</sub> emissions, suggesting that changes in Western lifestyles and a decrease in consumption may have a greater impact on mitigating climate change. It is imperative to implement multidisciplinary policy strategies that take into account all the statistically significant variables. The mitigation efforts must focus on the key drivers of climate change, as, without a comprehensive approach, significant emission reductions will be challenging to achieve.

This work could be generalized by extending the FOSR to a quantile version, where the regression parameters vary according to the quantile of interest. This extension would allow modeling high quantiles and extreme values of CO<sub>2</sub> emissions and identifying their drivers. As an example, de Carvalho et al. (2021) have recently proposed such an approach,

and it would be interesting to adapt it to a functional framework. Another possible development is to generalize the  $AR(1)$  covariance structure to an  $ARH(1)$  structure, which accounts for heterogeneity in the temporal dependence. Additionally, nonlinear terms could be introduced for the regression coefficients to partially overcome the drawbacks of considering uniform differences between SSPs levels.

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