

# Estimating process-based model parameters from species distribution data

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1. Two main types of species distribution models are used to project species range shifts in future climatic conditions: correlative and process-based models. Although there is some continuity between these two types of models, they are fundamentally different in their hypotheses (statistical relationships vs cause-to-effect relationships) and their calibration methods (dependent vs independent of the species observed distributions).
2. One of the main limitation to the use of process-based models is the difficulty to parameterize them for a very large number of species. Our aim was to calibrate process-based models in the same way as correlative models, i.e. using the geographic distributions of species. We investigated the feasibility of using an evolutionary algorithm (called covariance matrix adaptation evolution strategy, CMA-ES) to calibrate these models. This method is well established in some fields (robotics, aerospace research, ...), but has never been used, to our knowledge, in ecology, despite its ability to deal with very large space dimensions. Using tree species occurrence data across Europe, we adapted the CMA-ES algorithm to find appropriate values of model parameters. We estimated simultaneously 27 to 77 parameters of two process-based models simulating forest tree's ecophysiology for three species with varying range sizes and geographical distributions. We compared the performance of CMA-ES to a commonly used Approximate Bayesian Computation (ABC) method.
3. CMA-ES provided parameter estimates leading to better prediction of species distribution than parameter estimates based on experts knowledge. It was more efficient than ABC, and provided better parameter sets for the same amount of computation time. Predictions of process-based models calibrated with CMA-ES were as good as predictions of more simple correlative models calibrated with standard optimisation algorithms. Our results also revealed that some model parameters and processes were strongly dependent, and different parameter combinations could therefore lead to high model accuracy.
4. CMA-ES is an efficient state-of-the-art method to calibrate process-based models with a large number of parameters using species occurrence data. Inverse modelling using CMA-ES is a powerful method to calibrate process-based parameters which can hardly be measured.

**Keywords:** calibration, evolutionary algorithm, cma-es, species distribution model, process-based model, trees

## Introduction

The speed and magnitude of projected climate changes are profoundly affecting species distributions, ecological communities and ecosystem processes, and numerous ecological systems are now approaching

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tipping points (Lenton *et al.* 2008; Barnosky *et al.* 2012; Steffen *et al.* 2018). Large uncertainties on the persistence and the resilience of ecosystems exist. Ecological forecasting has now become a critical tool for managers and decision-makers (Urban 2015), and robust predictive approaches are necessary to provide reliable projections of species geographic range shifts and ecosystems functioning (Mouquet *et al.* 2015). Forecasting the dynamics of ecological systems for the upcoming decades and centuries is very difficult, because ecological systems are extremely complex, influenced by a lot of factors and processes, and climatic conditions with no analogous in the recent past are forecasted to become common (Williams *et al.* 2007; Radeloff *et al.* 2015; Fitzpatrick *et al.* 2018). Ecological models have thus increased in complexity over the last 50 years, incorporating more and more processes described with various degrees of complexity depending on their objectives.

Nowadays, two main types of species distribution models (SDM) are used to project species range shifts in future climatic conditions: correlative and process-based models (Dormann *et al.* 2012). The vast majority of currently used SDMs are correlative: they seek to find statistical relationships between various environmental descriptors and species presence and absence. They assume there is an equilibrium between species distribution and environment (equilibrium postulate, Guisan & Thuiller 2005), and that species niche is stable over time (niche conservatism, Pearman *et al.* 2008). Most of them include a fairly large number of predictors (particularly in machine-learning approaches), and consider flexible transformations (linear, quadratic...) and interactions between them (Merow *et al.* 2014). Even though some authors advocate for “putting more biology into SDMs” (Higgins *et al.* 2012), parameters have no a priori defined ecological meaning (Dormann *et al.* 2012) and shape of response curves to environmental variables is generally not constrained based on biological considerations. Although these models are not always used correctly (Araújo *et al.* 2019; Santini *et al.* 2021), their flexibility makes them an important tool in predictive ecology (Mouquet *et al.* 2015). They have been widely used especially to generate species range projections under current and future climates (e.g. Guisan & Thuiller 2005). Nevertheless, their ability to accurately describe the effects of climate on species distributions has recently been questioned (e.g. Fourcade *et al.* 2018; Journé *et al.* 2020; Warren *et al.* 2021). For all these reasons, another kind of models has been developed. Process-based models aim to translate into mathematical equations our knowledge about the physiological and ecological processes involved in an organism’s life, such as growth, reproduction, survival, movement, and interactions with other livebeings. Process-based models take more time to develop and are more challenging to use, but they might provide greater comprehension of the complexity

of ecosystem dynamics and more robust projections in novel conditions (Evans 2012; Zurell *et al.* 2016; Singer *et al.* 2016; Urban *et al.* 2016). A wide variety of process-based models exists, from quite simple models (e.g. Kleidon & Mooney 2000) to much more complex ones (e.g. Dufrêne *et al.* 2005). They all rely on an explicit representation of causal relationships, with a direct biological interpretation (Connolly *et al.* 2017). The choices about the specific processes to include into the model are made based on theory, empirical observations and the objectives of the research, and modeler subjectivity may play an important role. One of the challenges is to build a model with the appropriate amount of complexity: a too simplistic model might be unrealistic whereas a very complex model could be far beyond our ability to understand it (because of interconnected mechanisms) and calibrate it. Each model relies on different hypotheses with its own balance of complexity, accuracy and parsimony - and thus different numbers of unknown parameters to calibrate. Generally, the parameter values are obtained both from field or laboratory observations and experiments made by the modelers themselves or already available in the literature, as well as from statistical inference for each modeled process using process-specific data.

Calibration (i.e. parameter estimation) is a fundamental step in the modelling process. It fixes the model in reality, and allow it to reproduce this reality with more or less success. The result of the calibration provides insights on the ability of the model to reproduce and explain the reality (model predictive power). Calibration of complex models such as process-based SDMs is time-consuming, and modelers are often challenged by the dimension of the parameter space, the complexity of the possible correlations among parameters, and the scarcity of observed experimental data to calibrate them. Parameter inference can be achieved through many methods which have been developed in the last decades. Most of them fall into two categories: Bayesian inference or maximum likelihood estimation. On one hand, Bayesian inference aims at estimating parameter posterior distribution while taking into account prior belief. On the other hand, maximum likelihood methods aim at finding the parameters that maximize the model goodness of fit, and are either deterministic (e.g. Nelder-Mead method) or stochastic (e.g. simulated annealing, evolutionary algorithms). One of the promising method to solve high-dimensional optimization problems is the Approximate Bayesian Computation (ABC), which is increasingly being used in ecological modelling (Csilléry *et al.* 2010 ; Beaumont 2010). ABC combines a computational efficient approximation of posterior distribution with the advantages of Bayesian parameter inference (including the quantification of parameter uncertainty), and is thus particularly useful when numerical evaluation of the likelihood function is computationally not possible. Recently, an other approach belonging to the evolutionary algorithm

family, called Covariance Matrix Adaptation Evolution Strategy (CMA-ES), has been proposed (Hansen & Ostermeier 2001). One of the advantage of CMA-ES is its ability to cumulate information over iterations in order to adapt its own parameters (in particular the covariance matrix), which makes it more robust to noise. CMA-ES is especially performant for non-separable problems (i.e. when the model parameters are dependent) and large search space. This method has been successfully applied in various fields such as aerospace (e.g. Collange *et al.* 2010), optics (e.g. Gagné *et al.* 2008), and robotics (e.g. Hill *et al.* 2020). CMA-ES is acknowledged to be one of the most efficient approaches in continuous black-box optimization (Hansen *et al.* 2010) but to our knowledge has never been used in ecology.

Here we explored the feasibility and interests of calibrating process-based SDMs with CMA-ES using species occurrence data as correlative SDMs do. We focused on two forest process-based models of varying levels of complexity to evaluate the ability of CMA-ES to calibrate such models and compare its performance relatively to the more widely used ABC method. The two models are PHENOFIT (27 to 36 parameters, Chuine & Beaubien 2001) and CASTANEA (77 parameters, Dufrêne *et al.* 2005). Each model also emphasizes different ecological processes: while PHENOFIT focuses on phenology and how it relates to survival and reproduction, CASTANEA focuses on carbon and water cycles. We aimed to assess the ability of CMA-ES to calibrate these process-based models, to identify the limits of this method, and to compare its efficiency with an ABC algorithm commonly used among ecologists. To this end, we calibrated the models in the same way as correlative models do (fitted process-based models *sensu* Dormann *et al.* (2012)), that is to say, using the geographic distributions of species, and compare their efficiency to that obtained with classical calibration, i.e. direct measurement of the parameters or statistical inference of the different submodels using data for each modelled process. We focused on three European common tree species, with different range extent and ecological preferences in order to evaluate the algorithms performance in various geographical and climatic conditions. European beech (*Fagus sylvatica* L.) is one of the most widely distributed broadleaved tree in Europe (from southern Sweden to Sicily and from Spain to northwest Turkey), holm oak (*Quercus ilex* L.) is an evergreen broadleaved tree native of the Mediterranean region, and silver fir (*Abies alba* Mill.) is a coniferous tree which mainly occurs in mountain forests of Central Europe and some parts of Southern and Eastern Europe.

## 1. Material and methods

### 1.1. Process-based models

All versions of the models used for this study are coded in Java and distributed by the CAPSIS platform.

PHENOFIT is a process-based species distribution model for forest tree species which focuses on phenology. It relies on the principle that the distribution of a tree species depends mainly on the synchronization of its timing of development to the local climatic conditions (Chuine & Beaubien 2001). It is composed of several submodels, including phenology models for leaves, flowers and fruits, and stress resistance models. It simulates the fitness (survival and reproductive success) of an average individual using daily meteorological data, soil water holding capacity and species specific parameters (see Appendix A for details). PHENOFIT has been validated for several North American and European species by comparing their known distribution to the modelled fitness (e.g. Morin *et al.* 2007; Saltr  *et al.* 2013; Duputi  *et al.* 2015; Gauzere *et al.* 2020).

CASTANEA is an ecophysiological process-based model which simulates carbon and water fluxes in forests (Dufr ne *et al.* 2005). The model simulates the ecosystem as an average tree with six compartments (leaves, branches, stem, coarse roots, fine roots and reserves). It is much more complex than PHENOFIT, with several processes described and computed, such as photosynthesis, stomatal opening, maintenance and growth respiration, transpiration, and carbon allocation (see Appendix A for details). CASTANEA requires daily meteorological variables and soil characteristics. The model has been initially validated at stand scale for beech (Davi *et al.* 2005), and was then successfully applied to other European species (e.g. Davi *et al.* 2006; Delpierre *et al.* 2012; Davi & Cailleret 2017).

### 1.2. Data for the calibration

#### 1.2.1. Climate and soil data

Raw climatic variables were extracted from ERA5-Land hourly dataset (Mu oz Sabater 2019, 2021) from 1970 to 2000, at a spatial resolution of 0.1 degree in latitude and longitude. We calculated the daily mean values of the following variables used by PHENOFIT and CASTANEA: minimum, mean and maximum daily temperatures, mean dewpoint temperature, daily precipitation, daily global radiation and daily mean wind speed. We computed the daily relative humidity with the ratio of vapor pressure and saturation vapor

pressure (both calculated with Clausius-Clapeyron equation) using *humidity* R package (Cai 2019). Daily potential evapotranspiration was calculated with Penman–Monteith equation (FAO standard of hypothetical grass reference surface) using a slightly modified version of the *ET()* function in *Evapotranspiration* R package (Guo *et al.* 2016).

Water content at field capacity and wilting point data were extracted from EU-SoilHydroGrids (Tóth *et al.* 2017) which is at 1km resolution. Percentage of sand, silt and clay particles, percentage of coarse fragments, bulk density and soil depth were extracted from SoilGrids250m (Hengl *et al.* 2017) at a 250m resolution. These data (except for soil depth) are provided at seven soil depths, so we summarized them (weighted sum or weighted mean) taking into account each layer width and total soil depth. Finally, all variables were upscaled at the ERA5-Land spatial resolution 0.1°.

### 1.2.2. Tree occurrences in Europe

Sources of occurrence data are known to differ even for common European trees (Duputié *et al.* 2014) and this makes it quite challenging to gather comprehensive data at a sufficient spatial resolution all over Europe. The occurrence data we used essentially rely on the EU-Forest dataset (Mauri *et al.* 2017) which benefits from inventory and monitoring programmes implemented in most European countries. As EU-Forest is limited to forest ecosystems, we completed it with presence records extracted from the Global Biodiversity Information Facility (GBIF 2022, see Appendix B for all download links) but removing observations outside natural species ranges as defined by Atlas Flora Europae (AFE, Jalas & Suominen 1972–2005) and EuroVegMap (Bohn *et al.* 2003). By doing so, we also included occurrences of isolated native trees living outside forests, excluding records from arboreta or gardens where the species would have been planted as an exotic. For holm oak, we also added occurrence records in the Mediterranean Basin from the WOODIV database (Monnet *et al.* 2021), leaving out EU-Forest and GBIF records we had already gathered. We upscaled all species records at the ERA5-Land resolution (i.e. 0.1° cell, see 1.2.1. Climate data). We finally obtained 21458 occurrence cells for beech, 6653 for holm oak and 5385 for silver fir (see Appendix B for details).

All the datasets described above are presence-only data. Therefore, we generated cells where species are supposed to be absent, i.e. pseudo-absence cells. In order to avoid as far as possible creating false absence data, we used EU-Forest cells where the species is not reported present as pseudo-absence cells. We assumed that national forest inventories were exhaustive (which is not true since only specific forest

plots in a 0.1° cell are monitored). We obtained 25423 absence cells for beech, 37931 for holm oak and 38365 for silver fir (see [Appendix C](#)).

We selected subsets of 2000 points (1000 presences and 1000 pseudo-absences) in order to reduce computational costs. For each species, we generated ten presence clusters of similar bioclimatic conditions based on annual climate normals computed with R package *dismo* ([Hijmans et al. 2021](#)) and ERA5-Land variables. In each cluster, we randomly sampled a number of cells where the species is present proportional to the total number of a number of cells where the species is present in the cluster. The aim of this stratified random sampling was to make sure that all species environmental preferences were proportionally represented. We then randomly sampled the same number of pseudo-absence cells (see [Appendix B](#) for details).

### 1.3. Model calibration

#### 1.3.1. Covariance Matrix Adaptation Evolution Strategy principles

Covariance Matrix Adaptation Evolution Strategy (CMA-ES) is widely accepted as a robust optimization algorithm for non-linear, non-convex, as well as non-separated optimization problems in continuous domain ([Hansen & Ostermeier 1996](#); [Hansen & Ostermeier 2001](#); [Hansen 2006](#)). It is based on the principle of evolutionary biology, via recombination, mutation and selection of the most fit individuals (i.e. parameter sets providing the best predictions). At each iteration:

- $\lambda$  individuals are evaluated, i.e. model runs  $\lambda$  times with  $\lambda$  different parameter sets and the objective function is evaluated
- the best  $\mu$  individuals are selected
- the weighted mean individual  $m$  is computed (mean of the best  $\mu$  parameter sets weighted by their objective function value) - covariance matrix  $C$  and step size  $\sigma$  are updated (with information accumulated over several consecutive iterations)
- new  $\lambda$  individuals are sampled in a normal distribution  $\mathcal{N}(m, \sigma C)$ , with both recombination (via the favorite solution  $m$ ) and mutations (via the perturbations  $\sigma C$ )

One of the strength of this approach lies in the combination of rank- $\mu$ -update, where prior information from previous generations is exploited (mean of the previous covariance matrices, with a higher weight for recent generations), and cumulation, where correlations between generations are retained in an evo-



lution path (sum of consecutive steps), to update the covariance matrix at each step (see Hansen 2016 for a detailed description of the algorithm).

### 1.3.2. CMA-ES in practice

One of the advantages of CMA-ES is that it does not require a complex parameter tuning: as best parameter values at a given time of the optimization process might no longer be efficient later, CMA-ES implements an internal adaptation of its parameters. We only chose the population size  $\lambda$ , depending on the optimization problem complexity ( $\mu$  was set to  $\lambda/2$ ). The default recommended value for  $\lambda$  is  $4 + 3\ln(N)$ , where  $N$  is the number of parameters to calibrate (i.e.  $\lambda \in [14, 17]$  in our case). We set  $\lambda = 20$ , in order to improve the global search capability (Hansen & Kern 2004) and take advantage of the computation power at our disposal. All model parameters were linear scaled into  $[0; 10]$  so that the same standard deviation can be applied to all parameters: here we chose  $\sigma = 2$  (see Nikolaus Hansen personal website for practical hints on variable encoding). Our stopping criterion for the optimization procedure was the budget, i.e. the number of model runs.

For an easier use and the sake of reproducibility, we chose to use a pure R implementation of CMA-ES available in the R package *cmaes* (Trautmann et al. 2011). The function *cma\_es()* enables us to do  $\lambda$  function evaluations in parallel so as to substantially reduce computation time. It also allows us to define lower and upper bound constraints, by penalising individual fitness (i.e. objective function value) if it violates the boundaries. We customized the *cma\_es()* function to add an option to define death penalty constraints (rejection of the infeasible individual who is sampled again), in order to define a range of ecologically possible solutions in terms of inequality constraints between parameters (see Appendix D for details about boundaries and constraints handling). Death penalty is the easiest way to handle constraints when the feasible region is fairly large, but it is not perfect as there is no use of information from infeasible points.

In the spirit of species distribution modelling, the objective function for the calibration was the area under the receiver operating characteristic curve (AUC), evaluated against a subsets of 2000 points (see 1.2.2. Tree occurrences). Although AUC has been criticized as an imperfect measure of model performance (Lobo et al. 2008; Leroy et al. 2018), we used it as objective function because our goal here was only to calibrate models by maximizing discriminating capacity (i.e. potential to correctly classify presences and absences) with a threshold-independent measure. We used the *AUC* R package (Ballings & Van den Poel



Table 1: Summary of model calibration settings. Average runtime was assessed on the GenOuest cluster.

Model	Output variable of interest	Number of parameters calibrated	Population size $\lambda$	Number of cores	Memory	Average runtime
PHENOFIT	Fitness index	[27; 36]	20	40	80 Go	$\sim$ 24 hours
CASTANEA	Carbon reserves	77	20	100	120 Go	$\sim$ 20 days

2013), and chose the two following model output variables as proxies of classification probabilities (i.e. used to determine if the species can be present or not): fitness index for PHENOFIT and carbon reserves for CASTANEA (see Appendix A).

We implemented the CMA-ES calibration on two computing clusters: GenOuest from IRISA-INRIA ([genouest.org](http://genouest.org)) and TGCC (*Très Grand Centre de Calcul*) from CEA ([hpc.cea.fr](http://hpc.cea.fr)). As the models are coded in Java (see 1.1 Process-based models), they need a process of deallocating memory handled by a *garbage collector*. For PHENOFIT, each function evaluation (i.e. each model simulation) was run on a 2-core computing unit in order to have enough computing resources for both simulation and garbage collection. We thus needed twice as many cores as functions evaluated in parallel. CASTANEA model requires a fairly high computation time, so we used a nested parallelism distribution, where each parallel simulation was distributed on 4 computing units. We thus used 4 times as many cores as functions evaluated in parallel, plus some extra cores for garbage collection. We used R package *future* (Bengtsson 2021) for parallel processing.

Regarding PHENOFIT model, we calibrated ten times each species parameter set using CMA-ES algorithm, with 5 repetitions on 2 random subsets of presences/pseudo-absences (see 1.2.2. Tree occurrences), except for beech. In the latter case, we ran 10 repetitions on 10 subsets (i.e. 100 calibrations) to investigate both the effect of subsampling and the effect of stochasticity on the calibration performance of CMA-ES. Since CASTANEA computing time was much higher (see Table 1), we ran only two calibration for each species (on 2 different random subsets).

### 1.3.3. Approximate Bayesian Computation

In order to provide elements of comparison between CMA-ES and an other widely used and effective optimization algorithm, we also implemented an Approximate Bayesian Computation (ABC) method. We

chose ABC because it is well established in ecology (e.g. [Hartig et al. 2014](#); [Lagarrigues et al. 2015](#); [Vaart et al. 2015](#); [Gardner et al. 2020](#)). Several versions of ABC exist, but here we only explore the most accessible version, simple rejection. We chose this version because it does not require a tedious parameter tuning, and it is therefore as easy as CMA-ES to apply to various calibration problems. ABC rejection involves running the model a large number of times, with parameters randomly sampled from their prior distributions, and then accepting the simulations closest to the observed data. These retained simulations are then used to draw the posterior distributions of the model's parameters given the data. We used uniform priors with the same lower and upper bounds than CMA-ES. We ran the model the same number of times as CMA-ES (i.e. same number of objective function evaluations) and we obtain the same computation time. Therefore, we had a fair comparison of the performance of the two algorithms. We ran 30 ABC calibrations (10 repetitions on 3 subsets) of PHENOFIT for beech in order to be able to make a robust comparison with CMA-ES. To avoid getting a beech specific comparison, we also ran 10 ABC calibrations (5 repetitions on 2 subsets) of PHENOFIT for holm oak (see [Appendix E](#)).

## 2. Results

### 2.1. Calibration results

Calibrations using species distribution data, either CMA-ES or ABC, are thereafter called backward calibrations, and calibrations based on expert knowledge, observations and measurements of the processes modelled are called forward calibrations.

CMA-ES calibration of PHENOFIT model allows an average 17.2% increase of AUC across the three species compared to forward calibration ([Figure 1](#)). The maximum increase is obtained for silver fir, from 0.72 to 0.9 (25%).

CMA-ES calibration of CASTANEA allows an average 23.7 % increase of AUC compared to forward calibration ([Figure 2](#)), and a maximum increase obtained for holm oak (34.7%).

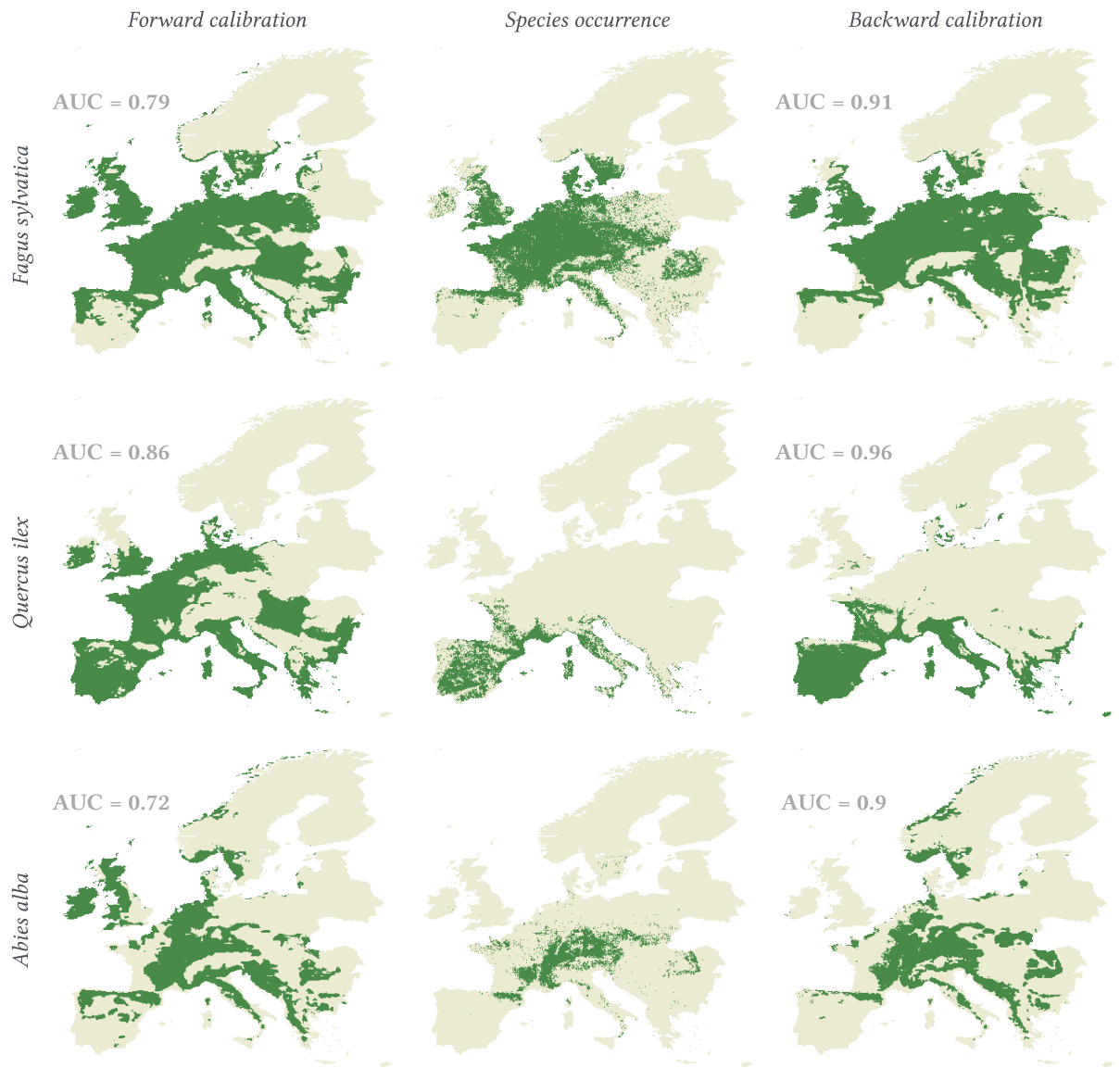


Figure 1: Species distribution maps obtained with PHENOFIT forward and backward calibrations, compared with observed species occurrences. Optimal threshold to dichotomize model predicted fitness index in presence/absence is the Youden index-based cut-off point. Note that models predict species climatic niche which is larger than the realized niche that corresponds to species presence map.

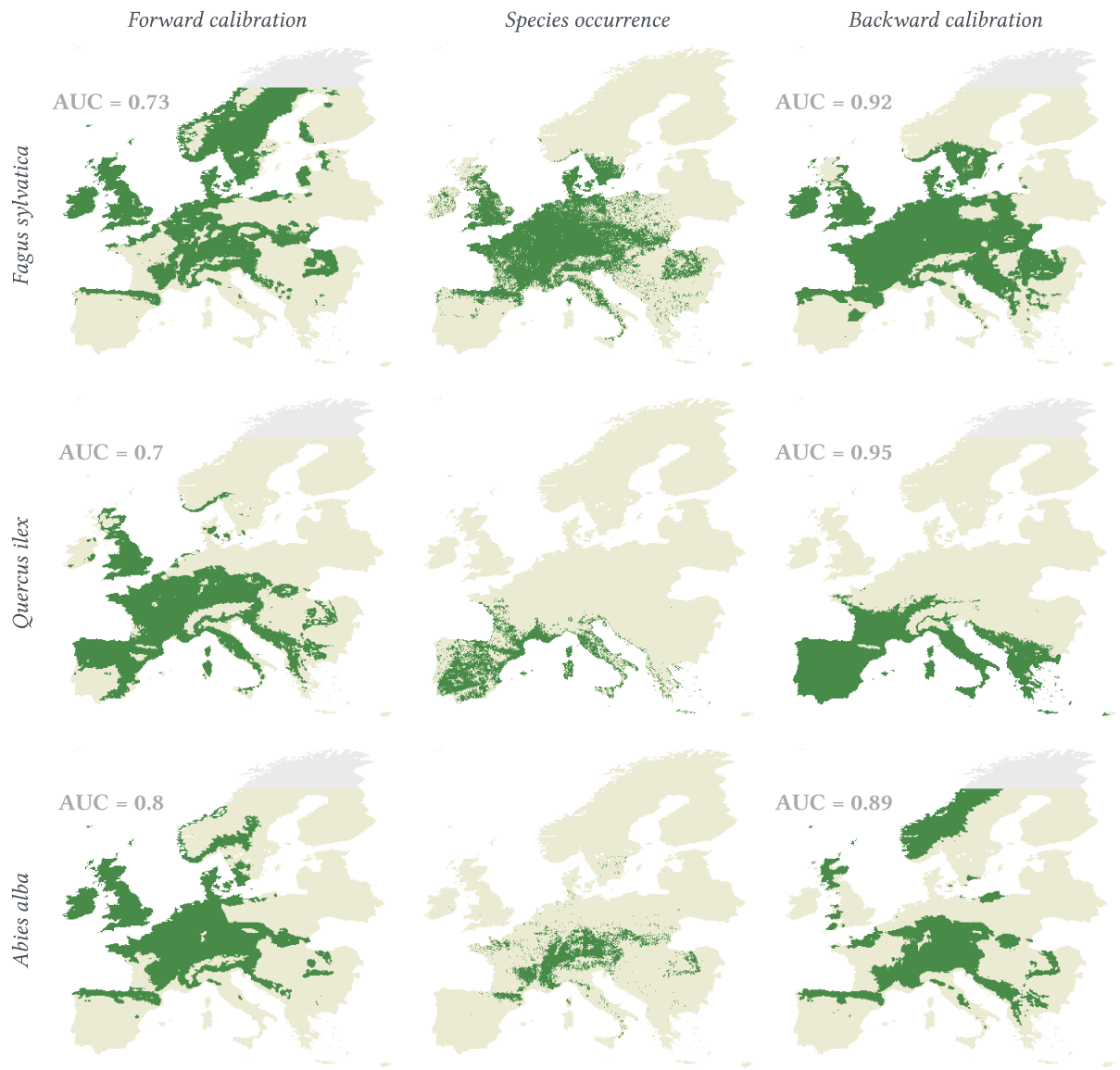


Figure 2: Species distribution maps obtained with CASTANEA forward and backward calibrations, compared with observed species occurrences. Optimal threshold to dichotomize model predicted carbon reserves in presence/absence is the Youden index-based cut-off point. Note that models predict species climatic niche which is larger than the realized niche that corresponds to species presence map.

## 2.2. Impacts of subsampling and calibration stochasticity

### 2.2.1. Variability of calibration performance

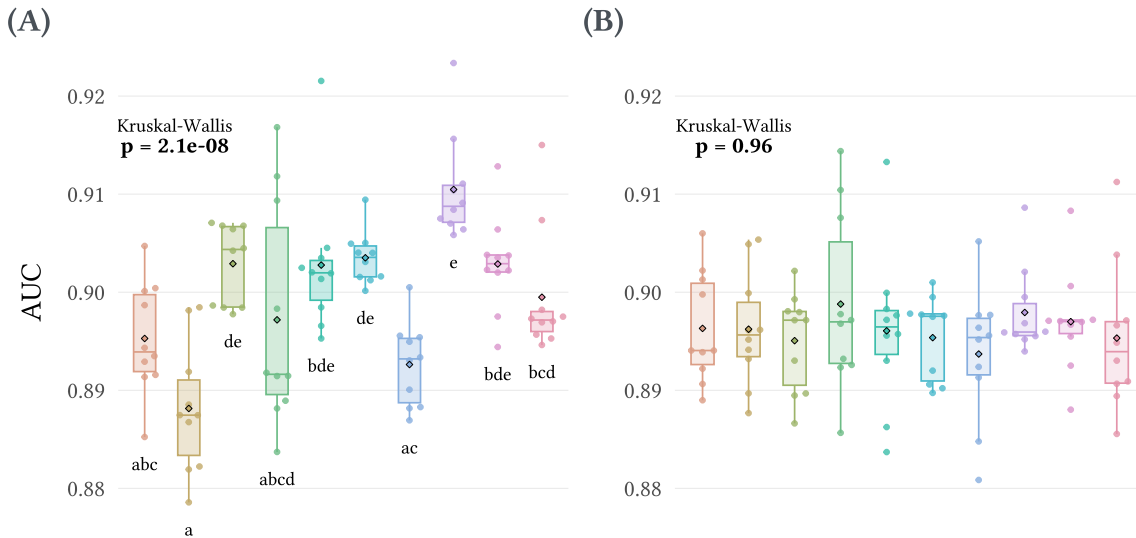


Figure 3: Effects of data sub-sampling and stochasticity on CMA-ES calibration using the PHENOFIT model for beech: **(A)** calibration AUC (calculated only with calibration cells) and **(B)** total AUC (calculated with all presence/absence cells). Each color is a different sub-sampling of occurrence data, each point is a calibration run. Diamonds (with black border) are mean AUC values. On **(A)**, the grouping letters represent the multiple comparisons with pairwise Dunn's tests.

The 100 calibrations of the PHENOFIT model realized for beech showed that random data subsampling had an effect on the final objective function value (i.e. the AUC computed on the 2000 calibration points). Kruskal-Wallis test was significant ( $p = 2.1e-08$ ), meaning that at least one subset provided better AUC during calibration. According to Dunn's tests, 11 pairwise comparisons out of 45 were significant (Figure 3.A.). The calibration AUC ranged from 0.879 to 0.923 over all subsets, with a mean value of 0.9.

However, more importantly, the repetition of calibrations on different subsets had no significant impact on the total AUC computed on all presence/absence points (Kruskal-Wallis test,  $p = 0.96$ ). Thus, no subset led to an overall better prediction of the species distribution (see Figure 3.B.). The total AUC ranged from 0.881 to 0.914, with a mean value of 0.896.

### 2.2.2. Non-identifiability of parameters

We found a high variability in the parameter estimates of the leaf unfolding date submodel of PHENOFIT after 100 calibrations (Figure 4.A.). For example, the critical amount of chilling  $C_{crit}$  required to break bud dormancy and the critical amount of forcing  $F_{crit}$  required to break bud ranged from 1.02 to 149.96 and from 1.5 to 79.26 respectively, with a mean value of 51.52 and 38.78. Their coefficient of variations were 126.7% and 51.9% respectively. Kendall correlation coefficient between  $C_{crit}$  and the threshold temperature of the response function to temperature during dormancy  $T_b$  is 0.64 ( $p < 0.001$ ). Kendall correlation coefficient between  $F_{crit}$  and the mid-response temperature  $T_{50}$  is -0.55 ( $p < 0.001$ ).

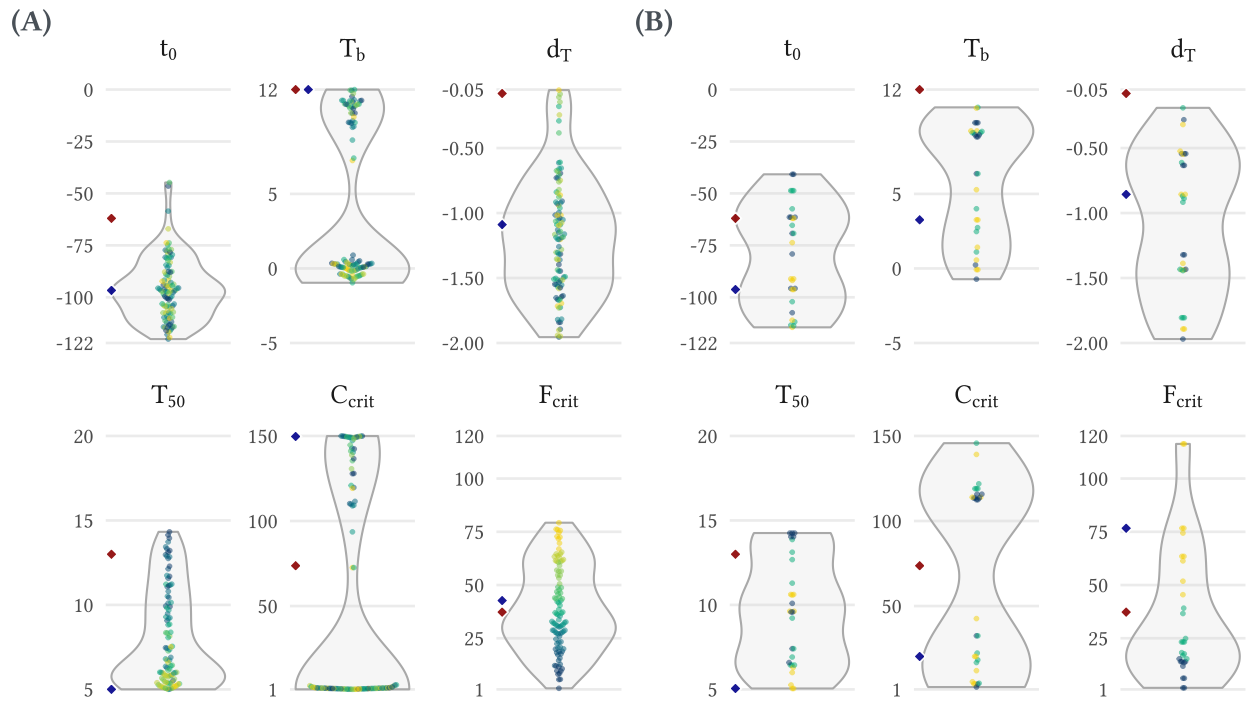


Figure 4: Effects of stochasticity of (A) CMA-ES and (B) ABC calibrations on PHENOFIT leaf unfolding model parameter values for beech. Y-axis limits are lower and upper bounds used during calibration. Each point is a calibrated parameter value, color gradient is based on  $F_{crit}$  values. Red diamonds are parameter values obtained with classical (forward) calibration, blue ones are parameter values obtained with the best backward calibration.

### 2.3. Comparing CMA-ES and ABC efficiency

The mean calibration AUC and total AUC obtained for beech with CMA-ES (0.899 and 0.896 respectively) were only slightly higher than those obtained with ABC (0.872 and 0.869). The best total AUC obtained with CMA-ES was 0.913, a higher value than the best solution obtained with ABC, 0.876. According to

Mann–Whitney tests, the distributions of AUC measures between the two methods with the three different occurrence subsets differed significantly (Figure 5). The outperformance of CMA-ES compared with ABC was the same for holm oak (see Figure E.1. in Appendix E). Both methods result in a high variability in the parameter estimates (Figure 4).

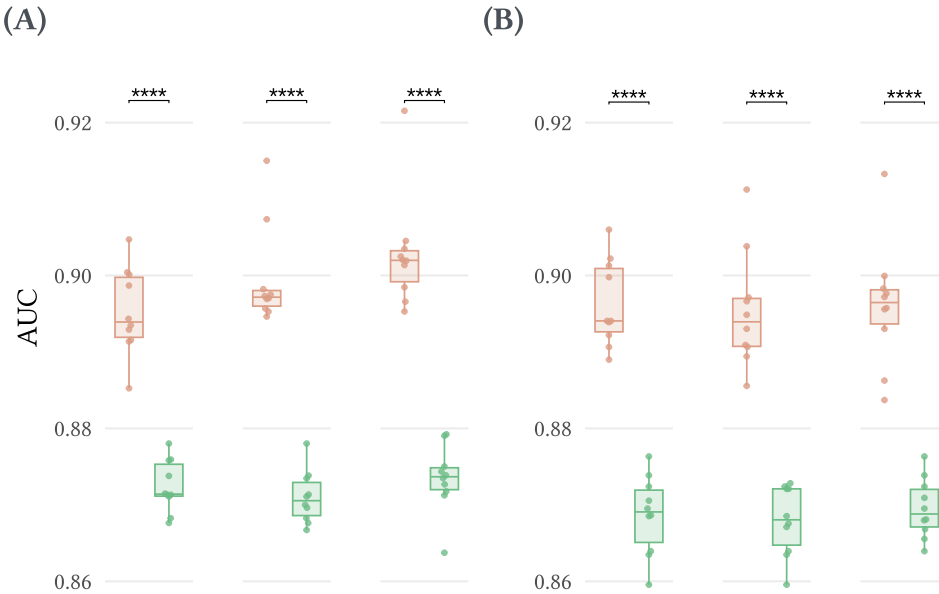


Figure 5: Comparison of CMA-ES and ABC-rejection methods, with three occurrence subsets of beech, on (A) calibration AUC (only calibration points) and (B) total AUC (every presence/absence points). Each point is a calibration run. The black horizontal bars represent the pairwise Mann–Whitney tests between the two methods on the same subset. CMA-ES is red and ABC green.

### 3. Discussion

#### 3.1. Performance and advantages of CMA-ES to calibrate complex models in ecology

Our results are the first to demonstrate that inverse calibration with CMA-ES is feasible and provide good results for complex and runtime-expensive ecological models.

With a subsampling of species occurrence data, the algorithm succeeds in finding parameter sets which provide high AUC values. The predictions of the calibrated models are sharply improved compared to classical (forward) parametrization (Figure 1 and Figure 2). AUC values obtained using CMA-ES were as good as the ones generally obtained with correlative models. Two striking examples are the increase in the performance of PHENOFIT model for silver fir, from 0.72 to 0.9, and of CASTANEA model for holm oak, from 0.7 to 0.95. Moreover, CMA-ES performed equally well regardless of the species occurrence subset



used during calibration (Figure 3.B.), and thus permitted to find a good compromise between computational cost and calibration efficiency.

CMA-ES is a “generic” optimizer which can be applied to various problems. It is easy to use as it does not require an extensive tuning to efficiently explore the parameter space. We only had to choose the population size  $\lambda$ , and the initial search region (initial starting point and step size  $\sigma$ ). As well as being quasi parameter-free, CMA-ES has several structural advantages:

- the covariance matrix allows to learn second-order information (pairwise dependencies between parameters)
- the covariance matrix adaptation is particularly efficient to deal with ill-conditioned and non-separable problems (Hansen *et al.* 2011)
- the update of the step size  $\sigma$  (i.e. mutation force) prevents premature convergence (Hansen & Ostermeier 2001)

CMA-ES has been shown to outperform several other optimization algorithms (Hansen *et al.* 2010), and is usually the most efficient method when the target cost (i.e. the number of objective function evaluations) is about  $100 * N$  ( $N$  being the dimension of the parameter search space, Bäck *et al.* 2013). Here we show that it outperforms the widely used ABC optimization method too.

### 3.2. Non-identifiability of parameter values

There can be a strong dependence between process-based model parameters.

In both models used in this study, biological mechanisms are explicitly calculated in several submodels (e.g. a leaf unfolding submodel or a stomatal opening submodel). A submodel output has inevitably a significant influence on the other submodels as biological processes can be highly dependent with feedbacks: in CASTANEA, for example, the stomatal opening affects the photosynthesis, and *vice versa*. Within each submodel, parameters are also strongly dependent because of structural correlations. To illustrate this problem, we focused on beech leaf unfolding submodel of PHENOFIT (see Appendix A). This model has 6 parameters (Chuine 2000): a starting date of the processes ( $t_0$ ), one parameter describing the response function to temperature during the dormancy phase ( $T_b$ ), two parameters describing the response function to temperature during the phase of bud growth ( $d_T$ ,  $T_{50}$ ), and two parameters representing the sums of the daily responses to temperature during bud dormancy ( $C_{crit}$ ) and during bud growth ( $F_{crit}$ ) that respectively determine the date of bud dormancy break and the date of leaf unfolding (see Appendix G for

details). Since no information on the date of bud dormancy break is available for the calibration, a first structural negative correlation exists between  $C_{crit}$  and  $F_{crit}$ : the same leaf unfolding date can be obtained with either a long dormancy phase and short bud growth phase or a short dormancy phase and a long bud growth phase. Other structural correlations exist between  $T_b$  and  $C_{crit}$  on the one hand and  $d_T/T_{50}$  and  $F_{crit}$  on the other hand: for example, a rapid accumulation of chilling units with a high critical chilling requirement could yield identical results as a slow accumulation with a low critical chilling requirement (i.e. the threshold temperature  $T_b$  and the critical chilling requirement  $C_{crit}$  are dependent, see Figure G.1.A. in [Appendix G](#)).

Consequently, several parameter sets may be statistically equivalent and parameters non-identifiable. In fact, calibration repetitions gave diverging parameter values ([Figure 4](#)) while being efficient in distinguishing between species presence and absence (i.e. AUC  $\sim$  0.9, [Figure 3](#)). Thus, even if the calibrated model describes the observed species distribution very well, it does not necessarily mean that parameter values are ecologically relevant. This concern is similar to the criticisms against correlative SDMs, in which parameter values and correlations that well reproduce species ranges not necessarily describe a complex biological reality. In our case, the constraints imposed by the explicit mathematical equations embedded in our models were not sufficient to ensure calibration convergence towards similar solutions that would have suggested a high biological realism. However, it is worth noting that we deliberately chose large parameter ranges (although biologically realistic, i.e. corresponding to the observations made on the different processes modelled across different species) in order to give free rein to the optimization algorithm. As our goal was to assess the performance of CMA-ES objectively, we did not attempt to minimize this non-identifiability issue by restricting the parameter space.

### 3.3. Methodological issues and perspectives of our study

Our goal here was to investigate the performance of CMA-ES to calibrate quite complex process-based species distribution models using species occurrence data. We did not attempt to validate our parametrizations using independent data, and AUC was only used to determine if model outputs were consistent with species distributions. However, AUC is scale-invariant (it measures how well predictions are ranked rather than their absolute values), and prevents us from obtaining calibrated outputs with more ecological meaning. For example, in PHENOFIT, one species with a fitness of 0.8 could be considered as absent whereas another one as present. Further work could thus be conducted to examine the effects of choosing a different

objective function.

We compared CMA-ES with a fairly simple but frequently used ABC algorithm because it is widely recognized as an efficient method, and has several advantages including its relative methodological simplicity (which makes it quite easy to implement) and its ability to quantify the uncertainty of the parameters. We did so to provide elements of comparison in order to evaluate CMA-ES performance, and we did not aim to argue for the merits of one approach over another. Higher computational efficiency might be obtained using other types of ABC algorithms, such as Sequential Monte Carlo (Beaumont 2010).

It would also be valuable to use a significantly higher computing power, with an adapted version of CMA-ES. To improve the global search performance of CMA-ES, we slightly increased the population size  $\lambda$  (Hansen & Kern 2004) and used a computing cluster to evaluate  $\lambda$  functions in parallel. We were able to use between 40 and 120 cores, which is far from the computing power of some GPUs (> 2000 cores). In this case, choosing a very large population size might not be the best choice. To use efficiently this large parallel computing power, one could rather use a CMA-ES restart strategy (e.g. IPOP-CMA-ES, Auger & Hansen 2005), where population size is successively increased (by a factor of 2), and run these calibrations in parallel. Moreover, when a model requires a high computation time and thus only a small budget can be afforded, the original fitness function could be approximated with a surrogate model in order to reduce the number of original function evaluations required (e.g. Auger *et al.* 2004 ; Loshchilov *et al.* 2013).

Finally, several authors advocate for process-based modeling approaches relying upon species response functions that are a priori defined (e.g. Higgins *et al.* 2020). However, the main limitation of such models is the data availability to infer their parameters (Urban *et al.* 2016). Forward parametrization is often long and arduous, and we demonstrated that CMA-ES backward parametrization of PBMs can be a powerful technique. One possible way to facilitate parameter values estimation would be to use backward calibration. In particular, CMA-ES driven by species occurrence data could be used to calibrate submodels whose parameter values can hardly be experimentally measured. However, when a structural correlation exists (as in the leaf unfolding submodel), backward calibration might not provide the right parameter estimates. In such a case, observations and measurements are necessary to determine *a posteriori* which estimates are the most realistic. A combination of both forward and backward calibrations might offer a new perspective for spreading the use of process-based models in predictive ecology, especially for climate change impact studies.

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## Conflict of interest

The authors have no conflicts of interest to declare.

## Author contributions

I.C. devised the main conceptual ideas. V.V. worked out the technical details, performed the numerical calculations and wrote the first draft of the manuscript. The two authors discussed the analyses and the results, and contributed to the final manuscript.

## Data availability

ERA5-Land dataset is available on the [Copernicus Climate Change Service website](#). EU-SoilHydroGrids is available on the [European Soil Data Centre website](#). SoilGrids250m is available on the [International Soil Reference and Information Centre website](#). EU-Forest database is available on [FigShare](#). The R code associated with this work will be made available on GitLab upon acceptance of the manuscript.

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