Oracle-Based Optimization Applied to Climate Model Calibration

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Abstract

In this paper, we show how oracle-based optimization can be used effectively for the calibration of an intermidiate complexity climate model. In a fully developed example, we estimate the 12 principal parameters of the C-GOLDSTEIN climate model by using an oracle-based optimization tool, Proximal-ACCPM. The oracle is a procedure which finds, for each query point, a value for the goodness-of-fit function and an evaluation of its gradient. The difficulty in the model calibration problem stems from the need to undertake costly calculations for each simulation and also from the fact that the error function used to assess the goodness-of-fit is not convex. The method converges to a 'best fit' estimate over ten times faster than a comparable test using the ensemble Kalman filter. The approach is simple to implement and potentially useful in calibrating computationally demanding models based on temporal integration (simulation), for which functional derivative information is not readily available.

Keywords: oracle-based optimization, cutting plane method, model calibration, parameter estimation, C-GOLDSTEIN, Proximal-ACCPM.

1   Introduction

The objective of this paper is to show how oracle-based optimization can be used effectively in model calibration for intermediate complexity climate models. Following [1], *model calibration* is defined as (i) the estimation of the model parameters to obtain the best match between observed and simulated behaviour of the phenomena described (*parameter estimation*) and (ii) the assessment of these *estimates* by confidence intervals (*estimate assessment*).

Climate models are playing a central role in the scientific debate concerning anthropogenic climate change, as indicated, for example, in the IPCC (Intergovernmental Panel on Climate Change)

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reports [2, 3]. These models are used to simulate the earth system response to the temperature forcing due to anthropogenic emissions of greenhouse gases. They include descriptions of atmoshere, ocean, ice and snow cover and precipitation dynamics in different locations on the planet. Model calibration is a vital issue in climate and earth system modelling since even so-called intermediate complexity models, such as the one used in this paper, can have a large number of uncertain parameters. More complex models, generally speaking, have correspondingly more, while simpler models typically have fewer parameters, but correspondingly greater uncertainty in their values. For climate prediction, in contrast to short-term weather prediction, parameter values, rather than initial conditions, are considered to be the dominant source of uncertainty. This may be true even for the ocean because interior processes are poorly understood or quantified, even though initial conditions are forgotten only over millenia.

[1] distinguishes two approaches for model calibration: *optimal filtering* and *model reference optimization*. In optimal filtering approaches, as for example the *ensemble Kalman filter* (EnKF) approach proposed by [4], the parameter estimation and the estimate assessment problems are treated simultaneously. These methods require some probabilistic assumptions concerning the prior distribution of unknown parameters and the model measurement errors (represented by a covariance matrix). In model reference optimization approaches the parameter estimation is done in a first step, followed by a second step concerning the estimate assessment. In the parameter estimation step the objective is simply to find the parameter values that minimize an *error function* (typically weighted least squares) in order to get the best fit between observed and simulated data. No *a priori* probabilistic information is assumed at this stage. In the estimate assessment step, confidence intervals for the parameter estimates can be determined by performing sensitivity analysis of the minimized error function [1].

We may see the model reference optimization approach, applied to a climate model, as an instance of a *design problem* where one has to choose the values for static parameters that influence the performance of a complex dynamical system. The difficulty lies indeed in the non-explicit link that exists between the static design parameter values and the evaluation of the dynamic system performance. In this paper we propose to use an oracle-based optimization tool (OBOT), namely Proximal-ACCPM, i.e, the *proximal analytic center cutting plane method* [5], to deal with this difficulty. An OBOT proceeds through a sequence of queries where an *oracle* replies by sending information about the performance indicator value and its gradient w.r.t. design parameter values. We demonstrate the potential of the method by performing parameter estimation for C-GOLDSTEIN [6] which is a simplified physics, low-resolution climate model, with a 3-D ocean, a 2-D atmosphere and a dynamic and thermodynamic sea-ice component. In this paper, we describe how the parameter estimation step has been performed using an OBOT. The extension to estimate assessment via sensitivity analysis will be the subject of another report.

We will compare our results to those reported by [6], where the C-GOLDSTEIN model has been calibrated using an EnKF method.

The paper is organized as follows: In section 2 we briefly introduce the C-GOLDSTEIN climate model. In section 3 we discuss the potential of Proximal-ACCPM for climate model calibration. In section 4 we formulate the minimization problem used to estimate the C-GOLDSTEIN parameters. In section 5 we briefly introduce Proximal-ACCPM. In section 6 we give the implemention details. In section 7 we report the results and finally, conclusions are given in section 8.

2 C-GOLDSTEIN

2.1 The model

In the hierarchy of climate and earth system models, C-GOLDSTEIN is of intermediate complexity. Owing to a combination of low spatial resolution and simplified physics, the model achieves an integration speed of one or two thousand years per hour on a modern PC (Pentium-IV, 2.4 GHz), thus it is three or four orders of magnitude (o.o.m.) more computationally efficient than widely used high-resolution GCMs such as HadCM3 [7], and one or two o.o.m. faster than other intermediate complexity models with three-dimensional ocean components such as ECBILT-CLIO [8] or the UVic model [9]. On the other hand C-GOLDSTEIN is an o.o.m. slower than the reduced dimensionality Bern 2.5-D model [10].

The oceanic momentum budget is represented by a simplified frictional geostrophic balance which is approximately valid for long timescales, of years to decades or more, and large spatial scales, of order 1000 km or more. The detailed dynamics of oceanic eddies, for instance, are neglected. The atmosphere has a single layer so that atmospheric processes are represented by a balance of energy and moisture plus simple horizontal transport by anisotropic diffusion and advection by a fixed wind field. Feedbacks involving changes in atmospheric circulation and precipitation patterns, and feedbacks involving the land surface, are therefore relatively poorly represented or ignored. Sea-ice height and areal coverage are similarly governed by a local heat and fresh water balance, plus advection by surface currents with a diffusive term to represent unresolved processes. For the studies described here, the ocean component is configured with 8 vertical levels while all components share the same 36 by 36-cell horizontal grid.

Processes relevant to global-scale ocean circulation are reasonably well represented by this version, as shown by [6]. As a result of its efficient but relatively faithful representation of large-scale ocean dynamics, the model has proved useful for studies of glacial circulation states [11], integrated assessments of climate change impacts [12] and parametric investigations of the stability of the thermohaline circulation [13]. The model is described more fully in [14]. C-GOLDSTEIN forms a component of the Grid Enabled Integrated Earth System Model (GENIE) project (www.genie.ac.uk) in the context of which an Earth System Model with more detailed representations of atmosphere, land-ice, ocean biogeochemistry and land-surface processes is under development.

2.2 The parameters

C-GOLDSTEIN contains a total of around 75 physical and model parameters, a subset of 12 of which were identified in [14] as the principal adjustable parameters governing transport and mixing, and thus the large-scale distributions of climatic variables (temperature, humidity etc). Even where these parameters correspond to well-defined physical processes which may, in principle, be measurable, the correct physical values remain hard to ascertain experimentally. Further, even where an appropriate true global average value could be tightly constrained by measurements, it may be appropriate to allow the model value to deviate from the measured bounds if this allows the model dynamical system to better approximate the real climate, in some desired averaged sense.

Thus in [14], an averaged error function is defined which measures the mean square departure

of the model state from observations. Good estimates of the 12 parameters are found by mini-mizing the error, over an ensemble of 1000 randomly chosen parameter sets within a predefined range. To better compare estimation results, exactly the same optimization problem, using the same data, the same cost function and, as far as possible, the same prior ranges, were addressed both in the present work and in the EnKF study of [6]. However, the prior information and the cost are treated somewhat differently by [6] as noted below. The observational data correspond to ocean and surface atmospheric statistics averaged over a period of around 50 years. Although there has been significant change in upper ocean and atmosphere temperatures over this period, these changes will be small relative to the error in such a simple model. Indeed, the error function essentially tests how well the model can reproduce the spatial distributions of atmospheric and oceanic variables. Since sources of internal variability such as eddies are not represented, the model typically responds to the steady imposed solar forcing used here by a slow approach toward a steady state. Physically, then, we consider this steady state as a representation of the preindustrial climate and wish to choose parameters which minimize the deviation between the steady state and the data.

3   Potential of Proximal-ACCPM for climate model calibration

In this section we briefly review possible alternatives for performing model calibration and we indicate why we believe an OBOT such as Proximal-ACCPM is well suited to this task.

As indicated in the introduction, model calibration has been attempted via two main strands of approaches; those related to *optimal filtering*, represented by the Kalman filter family of methods, and *model reference optimization.* The Kalman filter can be seen as a recursive *predictor-corrector* method [15] that was initially designed to estimate the state of a stochastic linear dynamical system. By starting at an initial guess of the system state and of the error covariance matrix and after some predictor-corrector iterations, the Kalman filter outputs an optimal estimated state and its associated error covariance matrix. The Kalman filter supposes an underlying linear system that at each iteration *predicts* the future state. Furthermore, at each Kalman filter iteration the state prediction and its associated error covariance matrix, are *corrected* by incorporating the measured information. Both linear system and measurements have associated noise functions which are assumed white and Gaussian.

A powerful variant of the Kalman filter suitable for non-linear systems is the *Ensemble Kalman Filter* (EnKF), introduced by [16]. The EnKF is based on an ensemble (set) of model states instead of a single model state (in contrast with the Kalman filter). As pointed out in [15], the EnKF can be interpreted as a statistical Monte Carlo method where the ensemble of model states evolves in the state space with the mean as the best estimate and the spreading of the ensemble determining the error variance. In the Kalman filter the stochasticity of the system state is completely represented by the estimate itself and the error covariance matrix. In contrast, in the EnKF, the stochasticity is approximately represented by the estimate itself and a cloud of points around it (ensemble of system states).

The Kalman filter is also used for parameter estimation (model identification). [17] shows how to implement the EnKF for this purpose. The technique consists in extending the definition of the state vector so as to include the model parameters (see [18]). [6] report on a calibration of the C-GOLDSTEIN model using the EnKF technique. This study showed a great improvement in computational efficiency compared to simpler Monte-Carlo parameter estimation techniques,

but the calculation was still relatively expensive, requiring 54 model runs, each of around 10,000 years (several times the model's intrinsic adjustment timescale). A critical detail of the method was that the model state and model parameters were treated differently in the iteration, in that the prior estimates for the model state were continually updated while the prior estimates for the parameters were not. This constrains the parameters to remain relatively close to the mean of the original, Gaussian parameter distributions.

In model reference optimization approaches one must first decide on the error function f to be minimzed. A common choice is weighted least squares which can be related to the maximum-likelihood method under appropriate assumptions on the distribution of errors [1]. To minimize the error function one may use zero-order methods, which only require evaluations of f, first-order methods which require also the evaluation of the gradient g and second-order methods which ask in addition for the evaluation of the Hessian H. In [19], zero-order methods (genetic algorithms, controlled random search, etc.) are used to calibrate different models arising in water industry systems. In this implementation the number of function evaluations is of the order of several thousands. In [20] a second-order method based on the Broyden-Fletcher-Goldfarb-Shano (BFGS) method is used to calibrate three parameters of a soil constitutive model. In this application only three parameters had to be estimated and the number of calls to the function evaluation was of the order of fifty to several hundreds.

Proximal-ACCPM is a cutting plane method which belongs to the class of first-order methods. In the C-GOLDSTEIN calibration problem, the only available functional information is the error function value f obtained at a high computational expense. The remaining functional information, g and H, when needed, has to be numerically computed by finite differences or automatic differentiation techniques. In our opinion, a first-order method represents *a priori* a good compromise when implemented through an algorithm like Proximal-ACCPM which keeps the number of oracle calls (defining the cutting planes) at a moderate level. Furthermore, most of the optimization methods are based on line search along an improvement direction, which requires extra function evaluations. In our case, the use of a method which is free of line search, like Proximal-ACCPM, is an advantage considering the very high computational cost of each function evaluation.

The main limitation of cutting plane methods is that in principle they are designed for convex optimization. Given that our error function shows non-convexities, we have adapted Proximal-ACCPM in order to deal with them. It is therefore important to note that we will not be able to guarantee that even a local optimum has been reached. However the method will provide solutions that improve the fit with observed data. We also note that global optimization methods [21], which are designed for non-convex functions, are computationally too demanding for this class of problems. Indeed these methods rely on enumeration schemes, like e.g. branch-and-bound methods, which usually result in a very high number of function evaluations.

4 The minimization problem

Our goal in this section is to formulate the parameter estimation minimization problem for the C-GOLDSTEIN model. For this purpose we characterize the modelled climate state by the vector $s \in \mathbb{R}^N$, which consists of the values of oceanic temperature and salinity and of atmospheric temperature and humidity at every model grid point. The minimization therefore does not explicitly consider velocity and sea-ice variables, but these are tightly linked to s by the model dynamics. Note that s corresponds to the steady state attained after a long integration and depends on twelve

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model parameters represented by x. Otherwise stated, for every possible vector of parameters x, C-GOLDSTEIN returns a vector $s(x)$. On the other hand, the real earth climate is represented by the observed state $S \in \mathbb{R}^N$. As error function we use the weighted mean square error

$$f(x) = \frac{1}{N} \sum_{i=1}^{N} \frac{(s_i(x) - S_i)^2}{\widehat{\sigma}_i^2}, \tag{1}$$

where the weight $\widehat{\sigma}_i^2$ is the variance associated to S_i, $i = 1, \ldots, N$. There is thus one value of $\widehat{\sigma}_i$ for each of the four physical variables, temperature and salinity in the ocean and temperature and humidity in the atmosphere. Both the variances and the mean error are calculated in computational space rather than physical space, i.e. unweighted by grid-cell volume, so that variables in regions of lower resolution do not carry greater weight. The error function is thus a balanced measure of how well the model succeeds in representing the quantities it attempts to represent.

Our parameter estimation problem searches for a set of parameters x^* that minimizes f over all allowed parameter sets and can be formulated as

$$\begin{aligned} x^* &= \arg \min f(x) \\ &\text{s.t.} \quad x \in D \subset \mathbb{R}^{12}, \end{aligned} \tag{2}$$

where the box domain D for the model parameters is defined by a lower and upper bound for each parameter x_i, that is,

$$D = [\underline{x}_1, \overline{x}_1] \times \ldots \times [\underline{x}_{12}, \overline{x}_{12}]. \tag{3}$$

The bound values can be found in Table 2.

As in any minimization problem a very important question is whether f is a convex function. However, the complexity of the C-GOLDSTEIN model prohibits us from determining the convexity of $f(x)$ analytically. As an heuristic approach, we can plot slices of the graph of $f(x)$ along the coordinate axes, i.e. we can plot $\phi_i(\alpha) = f(x^0 + \alpha e_i), i = 1, \cdots, 12$, where $e_i = (0, \ldots, 1_i, \ldots, 0)$ is the ith canonical vector of $\mathbb{R}^{12}$ and x^0 is the central point of the domain D. We have encountered convex and non-convex plots (see Fig. 1-2) thus f is clearly not a fully convex function. Similar, single-parameter bifurcation experiments were conducted by [14] for all 12 parameters. Most yielded convex graphs, but parameters controlling the global hydrological cycle in particular, such as atmospheric humidity transport, showed evidence of non-convexity associated with hysteresis and bifurcations between contrasting global ocean circulation states. We discuss this matter later. The second main difficulty is that each evaluation of f takes about 2.5 hours on a modern PC (Pentium-IV, 2.4 GHz.), since for any set of parameters x, $f(x)$ is obtained after a long simulation.

5   Proximal-ACCPM

To solve (2) we use Proximal-ACCPM (proximal analytic center cutting plane method), an effective and robust cutting plane method [5]. In its iterations, Proximal-ACCPM produces an outer polyhedral approximation of the function epigraph[1]. This approximation serves to delineate a localization set which contains the optimum. For convex optimization problems, the localization

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[1]The set of points that lie on or above the graph of a real-valued function, that is, the set of points $(x, z) \in \mathbb{R}^{n+1}$ such that $z \geq f(x)$.
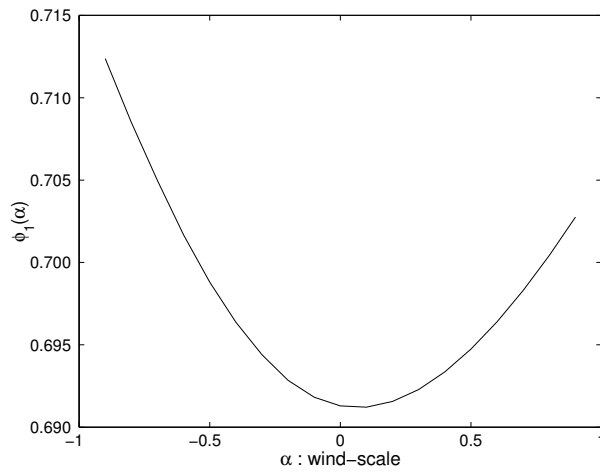
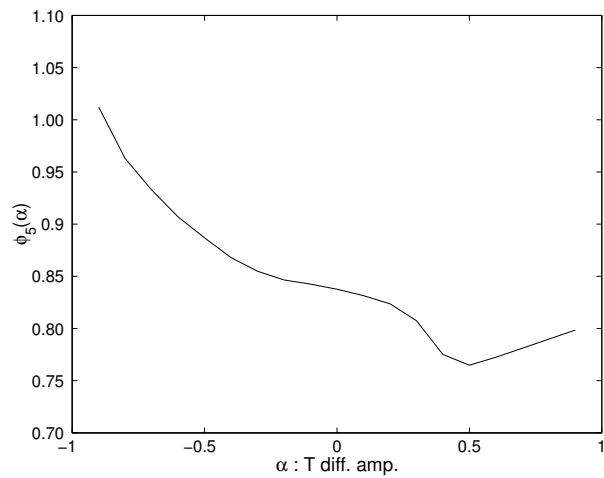Figure 1: Evolution of f(x) along the wind-scale parameter direction

Figure 2: Evolution of f(x) along the T. diff. amp. parameter direction

set rapidly shrinks to yield an optimal solution x^*. The role of Proximal-ACCPM is to efficiently guide the construction of such an approximation and eventually to find x^*. Proximal-ACCPM is a convex optimization tool and therefore must be applied with care when one deals with a non-convex problem as is the case here.

In the procedure, we consider a sequence of points $\{x^k\}_{k \in K}$ in the search domain D. We denote by g^k the gradient of $f(x)$ at x^k, that is, $g^k = \nabla f(x^k)$. We consider the linear approximation to $f(x)$ at x^k, given by $f^k(x) = f(x^k) + g^k \cdot (x - x^k)$ and have

$$f^k(x) \leq f(x)$$

for all x (to introduce Proximal-ACCPM we assume that f is convex).

The point x^k is referred to as a *query point*, and the procedure to compute the objective function and its gradient at a query point is called an *oracle*. Furthermore, the hyperplane that approximates the objective function $f(x)$ at a feasible query point and defined by the equation $z = f^k(x)$, is referred to as a *cut*.

An upper bound to the minimum value of $f(x)$ is provided by:

$$\theta_u = \min_k f(x^k).$$

The *localization set* is defined as

$$L = \{(x, z) \in \mathbb{R}^{12+1} \mid \quad z \geq f^k(x) \quad \forall k \in K, \quad z \leq \theta_u\}. \tag{4}$$

The basic iteration of a cutting plane method can be summarized as follows

1. Select $(\widehat{x}, \widehat{z})$ in the localization set L.

2. Call the oracle at $\widehat{x}$. The oracle returns one cut and a new upper bound $f(\widehat{x})$.

3. Update the bounds:

   (a) $\theta_u \leftarrow \min\{f(\widehat{x}), \theta_u\}$.

   (b) Compute a lower bound θ_l to the optimum of problem (2). For example, $\theta_l = \min\{z \mid (x, z) \in L \cap D\}$.

4. Update the upper bound θ_u and add the new cut in the definition of the localization set (4).

These steps are repeated until a point is found such that $\theta_u - \theta_l$ falls below a prescribed optimality tolerance. The initial domain is thus 'cut' down in size by the repeated removal of regions which cannot contain the optimum (given the assumption of convexity).

Cutting plane methods essentially differ in the way one chooses the query point. For instance, the intuitive choice of the Kelley point $(\widehat{x}, \widehat{z})$ [22] that minimizes z in the localization set may prove disastrous, because it over-emphasizes the global approximation property of the localization set. Safer methods, as for example bundle methods [23] or Proximal-ACCPM [5], introduce a regularizing scheme to avoid selecting points too "far away" from the best recorded point. Proximal-ACCPM selects the *proximal analytic center* of the localization set. Formally, the proximal analytic center is the point $(\widehat{x}, \widehat{z})$ that minimizes $F_\rho(x, z)$, defined as the logarithmic barrier[2]

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[2] The logarithmic barrier for the half space $\{x \in \mathbb{R}^n \mid a^T x \geq b\}$ is $-\log(b - a^T x)$.

of the localization set plus a quadratic proximal term which ensures the existence of a unique minimizer[3] for $F_\rho(x, z)$. This point is relatively easy to compute using the standard artillery of Interior Point Methods. Furthermore, Proximal-ACCPM is robust, efficient and particularly useful when the oracle is computationally costly —as is the case in this application.

6 Implementation details

6.1 Variable scaling

The bounds for the twelve parameters $\underline{x}_i$ and $\overline{x}_i$, that define D in (3), vary greatly from parameter to parameter (see Table 2) thus in order to optimize efficiently, x needs scaling. [24] propose a linear transformation of the form $x = T(y) = Ay + b$ where $A = [a_{ij}]$ is a diagonal matrix, $a_{ii} = 0.5(\overline{x}_i - \underline{x}_i)$, and $b_i = 0.5(\overline{x}_i + \underline{x}_i)$. In this case $T^{-1}(x)$ transforms domain D into $[-1, 1]^{12}$ and problem (2) is transformed into the following equivalent one:

$$
\begin{aligned}
y^* &= \arg\min \widehat{f}(y) \\
&\quad \text{s.t.} \quad y \in [-1, 1]^{12},
\end{aligned}
\tag{5}
$$

where

$$
\widehat{f}(y) = \frac{1}{N} \sum_{i=1}^{N} \frac{(\widehat{s}_i(y) - S_i)^2}{\widehat{\sigma}_i^2},
$$

and with $\widehat{s}(y) = s(T(y)) = s(x)$. Although in practice we solve the scaled problem (5), we will continue to use the simpler '$f(x)$' notation instead of '$\widehat{f}(y)$' for convenience.

6.2 Derivative approximation

Since it is not feasible to derive an analytical expression for $\nabla f(x)$, we approximate the partial derivatives by the forward-difference formula:

$$
\frac{\partial f(x)}{\partial x_i} \simeq \frac{1}{h}[f(x + he_i) - f(x)] \quad i = 1, \ldots, 12.
\tag{6}
$$

As we will see later, we only use approximate values $\widetilde{f}(x)$ instead of the true value $f(x)$. In this case, special care must be taken in the computation of the approximated partial derivatives [24]. Given that $\widetilde{f}(x)$ introduces an error $\delta(x)$, i.e., $\widetilde{f}(x) = f(x) + \delta(x)$, then we have

$$
\begin{aligned}
\frac{1}{h}[\widetilde{f}(x + he_i) - \widetilde{f}(x)] &= \frac{1}{h}[f(x + he_i) - f(x)] + \frac{1}{h}[\delta(x + he_i) - \delta(x)] \\
&\simeq \frac{\partial f(x)}{\partial x_i} + \frac{1}{h}[\delta(x + he_i) - \delta(x)], \quad i = 1, \ldots, 12.
\end{aligned}
$$

Thus, even for a small error $\delta(x + he_i) - \delta(x)$, we may obtain completely meaningless approximated derivatives for small values of h. In our computational experience this has been the case for $h \leq O(10^{-6})$ and best results have been obtained with $h = O(10^{-2})$ or $h = O(10^{-3})$.

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[3] That is, the proximal analytic center of L is the point

$$
(\widehat{x}, \widehat{z}) = \text{argmin}_{x,z} F_\rho(x, z) = \text{argmin}_{x,z} \{F_L(x, z) + \rho\|x - \widetilde{x}\|^2\},
$$

where $F_L(x, z)$ is the logarithmic barrier for the localization set L, ρ is the proximal weight, and $\widetilde{x}$ is the proximal point (current best point).

6.3 Coping with non-convexity

As already stated, Proximal-ACCPM is designed for convex problems. The convexity assumption is crucial in the convergence analysis of the method [25, 26], and even in its definition. Indeed the definition of analytic center applies to convex sets with a nonempty interior. The localization set that Proximal-ACCPM builds satisfies this assumption when the function to be minimized is convex. If the function is not convex, simple examples show that the oracle may produce cuts that totally exclude the current localization set. After adding the new cut, the set becomes empty and the method fails.

In our case, we know that the function we minimize is not convex. Indeed, we have observed that the oracle occasionally produces cuts that exclude a previously computed point, which, by construction, belongs to the epigraph set. To cope with the risk of an empty localization set, we use a simple device, based on the observation that the epigraph of a function is unbounded along the vertical axis. To ensure non-emptiness, we check whether a new cut excludes our reference point (the best point in the epigraph generated so far). If not, we proceed as usual, otherwise we lift the upper bounding cut by a sufficient amount.

This procedure is heuristic. It guarantees that the method does not unduly stop. However, we cannot guarantee that the point at which the convergence criterion of Proximal-ACCPM is met corresponds to a local minimum. We can only claim that we have empirical evidence on our climate problem that our simple heuristic device enables Proximal-ACCPM to converge to a point with low least-squares residual. This positive result is probably due to the fact that the function we minimize is only mildly non-convex, at least in the area of interest. Further enhancement of the Proximal-ACCPM technique would be required in order to guarantee convergence to a local minimum in non-convex cases.

6.4 Fast computing of the error function

We now consider how to accelerate the computation of the costly $f(x)$. The error function $f(x)$ is a continuous function of $s(x)$ whose definition is based on the integration of a system of partial differential equations along an infinite time horizon. If we define $\widetilde{s}(s^0, t, x)$ as the final state associated to an initial state s^0, an integration length t and a vector of system parameters x, then by definition $s(x) = \lim_{t \to \infty} \widetilde{s}(s^0, t, x)$ for any $s^0 \in S^0$, the set of suitable initial states of the dynamical system. (Note that we are assuming, for now, that $s(x)$ does not depend on the initial state s^0).

In practice, we have observed that with an integration length of 5000 years we obtain a very good approximation of $s(x)$ for a reasonable initial state s^0, i.e., $s(x) \simeq \widetilde{s}(s^0, 5000, x)$. The computing of $\widetilde{s}(s^0, 5000, x)$, takes about 2.5 hours on a modern PC (Pentium-IV, 2.4 GHz). At each iteration of Proximal-ACCPM we need to compute $f(x^k)$ and the approximation to $\nabla f(x^k)$ given by (6), which implies the evaluation of $s(x)$ at 13 points. This means that with this direct approach we need about 32.5 hours of CPU for each Proximal-ACCPM iteration.

An alternative to this direct approach is to use the so-called *warm start* procedure in C-GOLDSTEIN. Assuming, once again, that for two different initial states s^0 and s^1 we have

$$s(x) = \lim_{t \to \infty} \widetilde{s}(s^0, t, x) = \lim_{t \to \infty} \widetilde{s}(s^1, t, x),$$

we can accelerate the computing of, say $s(x^b)$, provided we already know $s(x^a)$ for an x^b close

to x^a. In this case $s(x^a)$ should not to be too far from $s(x^b)$ and therefore a short integration with $s(x^a)$ as initial state, should be enough to compute $s(x^b)$. That is,

$$s(x^b) \simeq \widetilde{s}(s^0, t_s, x^b) \simeq \widetilde{s}(s(x^a), t_w, x^b),$$

with $t_w << t_s = 5000$. $\widetilde{s}(s^0, t_s, x^b)$ and $\widetilde{s}(s(x^a), t_w, x^b)$ are respectively called the *standard start* and the *warm start* approximations of $s(x^b)$. Analogously, t_s and t_w are respectively called the standard start and warm start integration lengths.

The error function associated to $\widetilde{s}(s^0, t, x)$ is

$$\widetilde{f}(s^0, t, x) = \frac{1}{N} \sum_{i=1}^{N} \frac{(\widetilde{s}_i(s^0, t, x) - S_i)^2}{\widehat{\sigma}_i^2}.$$

By continuity, $\widetilde{f}(s^0, t, x)$ inherits the asymptotic behaviour of $\widetilde{s}(s^0, t, x)$. For example, it is easy to see that $f(x) = \lim_{t \to \infty} \widetilde{f}(s^0, t, x)$ for any $s^0 \in S^0$. Analogously, $\widetilde{f}(s^0, t_s, x^b)$ and $\widetilde{f}(s(x^a), t_w, x^b)$ are respectively called the standard start and the warm start approximations of $f(x^b)$.

To compute fast and reliable approximation to $f(x^k)$ and to $\nabla f(x^k)$, we use the warm start procedure as follows:

Central point warm start algorithm

1. *Warm start initialization:* Previous to any Proximal-ACCPM iteration, select $s^0 \in S^0$. Compute and store $\widetilde{s}^0 = \widetilde{s}(s^0, t_s, x^0)$ the standard start approximation of $s(x^0)$.

2. *Warm start:* At each Proximal-ACCPM iteration k compute and store

$$\widetilde{s}^k = \widetilde{s}(\widetilde{s}^{k-1}, t_w, x^k),$$

   approximate $f(x^k)$ by $\widetilde{f}(\widetilde{s}^{k-1}, t_w, x^k)$ and approximate $f(x^k + he_i)$ by $\widetilde{f}(\widetilde{s}^k, t'_w, x^k + he_i)$, $i = 1, \ldots, 12$.

3. *Partial derivatives:* Approximate partial derivatives $\partial f(x^k)/\partial x_i$ by:

$$\frac{1}{h}[\widetilde{f}(\widetilde{s}^k, t'_w, x^k + he_i) - \widetilde{f}(\widetilde{s}^{k-1}, t_w, x^k)] \quad i = 1, \ldots, 12. \tag{7}$$

4. *Accurate value of $f(x^*)$:* Once Proximal-ACCPM determines x^* as the best encountered point, approximate $f(x^*)$ by an extra standard start C-GOLDSTEIN call $\widetilde{f}(s^0, t_s, x^*)$.

Note that at step 2, at each perturbed point $x^k + he_i$ the warm start procedure uses the steady state attained when computing the objective function at the central point x^k. This approach takes advantage of the fact that the distance between any of these perturbed points and the central point is h. For this reason, at a perturbed point, by using the warm start procedure, the dynamical system recovers its steadiness after a very short integration length. This phenomenon can be intuitively observed in Fig. 3.

An alternative warm start approach could be as follows:

Parallel warm start algorithm

1. *Warm start initialization:* Previous to any Proximal-ACCPM iteration, select $s^0 \in S^0$. Compute and store $\widetilde{s}^{0,i} = \widetilde{s}(s^0, t_s, x^0 + he_i)$ the standard start value of $s(x^0 + he_i)$ for $i = 0, \ldots, 12$ (the vector e_0 being the null vector).

2. *Warm start:* At each Proximal-ACCPM iteration k compute and store

$$\widetilde{s}^{k,i} = \widetilde{s}(\widetilde{s}^{k-1,i}, t_w, x^k + he_i)$$

and approximate $f(x^k + he_i)$ by $\widetilde{f}(\widetilde{s}^{k-1,i}, t_w, x^k + he_i)$ $i = 0, \ldots, 12$.

Steps 3 and 4 would be as in the central point warm start algorithm. Obviously this approach is better suited for parallel computing than the previous one, since now the 13 C-GOLDSTEIN calls at step 2 are independent. The main drawback of the Parallel procedure is that it does not take advantage of the proximity between the central and perturbed points when computing the approximation to the partial derivatives (see next section). Since we are using a single processor PC, this is the reason why we have chosen the central point warm start in this paper.

6.5   Selection of the integration length

The critical parameter in our method is the integration length in the C-GOLDSTEIN model. A long integration will result in accurate results but long computations. A too short integration will produce the opposite effect. Our aim is therefore to find an integration length which balances both computation time and accuracy. The selection of the integration lengths t_s, t_w and t'_w has been done in an heuristic way by observing the evolution of the climate state. The evolution of the climate state as a function of the time $\widetilde{s}(s, t, x)$, can be visualized by plotting the basin-averaged deep-water temperature in the model Atlantic (below ≈ 1000 m depth), $T_d(s, t, x)$

In Fig. 3, the left-hand plot corresponds to $T_0(t) = T_d(s^0, t, x^0)$ obtained by a standard start C-GOLDSTEIN call with initial state s^0 and x^0 as parameter vector. The initial state s^0 is a globally uniform state with warm water throughout the ocean, as used by [14]. We observe that the temperature stabilizes around 12.6^oC after 5000 integration years, i.e., $lim_{t\to\infty}T_d(s^0, t, x^0) \simeq T_d(s^0, 5000, x^0) = 12.6^o$C.

The central plot corresponds to $T_1(t) = T_d(\widetilde{s}^0, t, x^1)$ obtained by a warm start C-GOLDSTEIN call with initial state $\widetilde{s}^0 = \widetilde{s}(s^0, 5000, x^0)$ and x^1 as parameter vector. We observe that, by using the warm start, the temperature stabilizes around 13.15^oC after an integration period of only 1000 years, i.e., $lim_{t\to\infty}T_d(\widetilde{s}^0, t, x^1) \simeq T_d(\widetilde{s}^0, 1000, x^1) = 13.15^o$C.

The right-hand plot corresponds to $T_2(t) = T_d(\widetilde{s}^1, t, x^1 + he_1)$ obtained by a warm start C-GOLDSTEIN call with initial state $\widetilde{s}^1 = \widetilde{s}(\widetilde{s}^0, 1000, x^1)$ and $x^1 + he_1$ as parameter vector. We observe that, by using the warm start at a slightly perturbed point, the temperature stabilizes very quickly. In order to reduce the CPU time, the goal is to take integration lengths t_s, t_w and t'_w as short as possible but ensuring the steadiness of the C-GOLDSTEIN dynamical system in order to obtain well approximated values of f and its partial derivatives. From our numerical experience we have observed that good values for the integration times are: $t_s = 5000, t_w = 500$ and $t'_w = 50$. Furthermore, C-GOLDSTEIN routinely calculates a diagnostic parameter ROC which measures the root mean square rate of change of ocean variables and thus provides a very strong measure of unsteadiness. This can be used to guarantee the quality of our approximation to $f(x^k)$ in step 2 of the central point algorithm. After computing $\widetilde{f}(\widetilde{s}, t, x^k)$, a low value of the associated ROC ensures a good approximation to $f(x^k)$. In our implementation, whenever the ROC has been
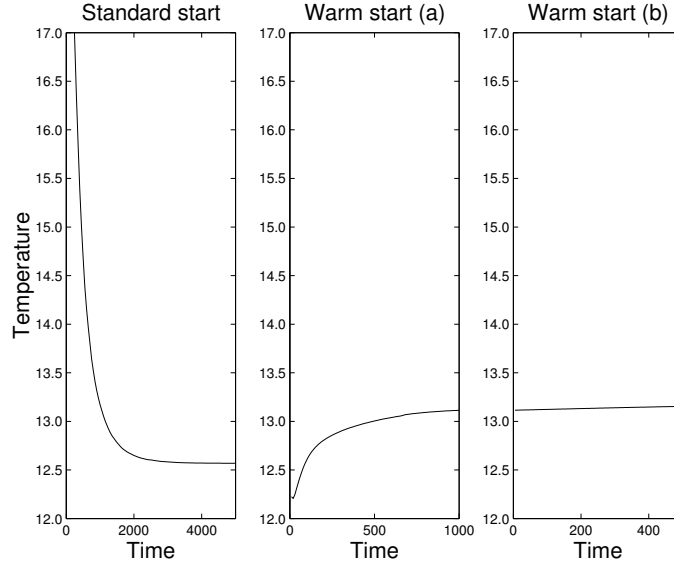
Figure 3: Deep-water temperature in the model Atlantic as a function of time for various initial states. Left-hand side plot: The standard start needs a long integration to attain a steady state. Central plot: The warm start needs a shorter integration to attain a steady state. Right-hand side plot: The warm start at a slightly perturbed point attains steadiness with a very short integration.

greater than 0.01, an extra integration has been performed in order to double the integration time and thus improve the approximation to $f(x^k)$. This last mechanism is seldom used and roughly speaking we can say that by using this warm start setting, at each Proximal-ACCPM iteration we divide by nearly 60 $(13 \times 5000/(500 + 12 \times 50))$ the standard start integration time per iteration, without noticeably increasing the number of Proximal-ACCPM iterations required.

7 Results

In this section we compare the results of our model calibration with those of the ensemble Kalman filter (EnKF) method, both from the numerical perspective and from the point of view of the resulting model climate.

7.1 Numerical performance

In our approach, we have used $h = 10^{-2}$ to estimate the derivatives (see Eq. (6)) and $\epsilon_{ACCPM} = 10^{-3}$ for the Proximal-ACCPM stopping tolerance. As initial point x^0 for Proximal-ACCPM we have taken the centre of the box domain D in equation (2). The initial state s^0 is globally uniform as noted above. Programs have been written in MATLAB 6.1 [27] and run on a PC (Pentium-IV, 2.4 GHz, with 6 Gb of RAM) under the Linux operating system. C-GOLDSTEIN is coded in Fortran 77.

Figure 4 shows the evolution of the Proximal-ACCPM upper and lower bounds up to convergence after 33 iterations. In the case of a convex error function the upper bound plot would be
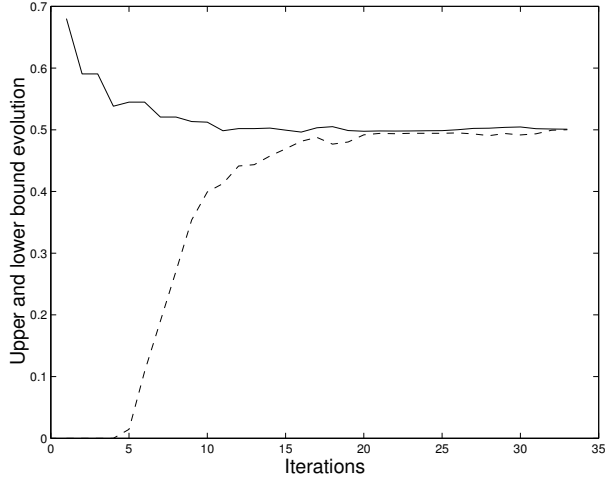
Figure 4: Proximal-ACCPM convergence.

Table 1: Performance. Note that the EnKF value corresponds to 10,000 years
per ensemble member and that the estimate referred to corresponds to the en-
semble mean, which may not be the lowest-error solution found.

Method	Lowest error	Integration length
EnKF	0.4944	540,000 years
Proximal-ACCPM	0.4896	47,000 years

monotonically non-increasing, that is, $\theta_u^k \geq \theta_u^{k+1}$ for all k. Here this is not the case due to the apparently mild non-convexity of f. As seen in Section 6, Proximal-ACCPM may lift the current upper bound in order to cope with the non-convex case.

Regarding the solution quality, Proximal-ACCPM finds a slightly lower function value of 0.4895 compared to 0.4944 for the EnKF approach (see Tables 1-2). Regarding the performance, the more reliable integration length (as opposed to the CPU hours) was used to compare the two methods. Proximal-ACCPM converges after 33 iterations, when the relative gap between the upper bound (objective function) and the lower bound falls below the stopping threshold ϵ_{ACCPM} (see Fig. 4). The total number of integration years for Proximal-ACCPM after 33 iterations was: 5000 years for the warm start initialization, plus $33 \times (500 + 12 \times 50)$ for the Proximal-ACCPM iterations (warm start), plus 700 integration years to improve the ROC parameter in a few cases plus 5000 integration years to compute the exact value of the error function at the optimal point. All in all, we needed 47000 integration years compared to around $54 \times 10,000 = 540,000$ integration years for the EnKF method, as reported in [6]. The overhead CPU times for Proximal-ACCPM and the EnKF methods are both considered negligible compared to the climate integration times. For the computer we have used, the reported integration lengths would correspond to estimated CPU times of 270.0 and 23.5 hours for EnKF and Proximal-ACCPM methods, respectively. It should be noted that the large amount of data processed in the EnKF method can lead to further computational overheads, but on the other hand the EnKF computation can be parallelised, corresponding to a minimim integration time of 5 CPU hours per node across 54 nodes. In contrast to the results obtained by EnKF and Proximal-ACCPM, the latin hypercube Monte Carlo method of [14], required 2,000,000 integration years but failed to locate any solutions with error less than 0.6000.

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Table 2: Estimated parameters.

	Parameters	Bounds		Estimated parameters		Units
	Ocean	Lower	Upper	EnKF	Proximal-ACCPM	
1	Wind-scale	1.0e+0	3.0e+0	1.6674e+0	1.1841e+0	-
2	Isopyc. diff.	3.0e+2	1.0e+4	4.1264e+3	5.5321e+3	$m^2 \, s^{-1}$
3	Diapyc. diff.	2.0e−6	2.0e−4	1.8134e−5	3.8818e−5	$m^2 \, s^{-1}$
4	Friction^{-1}	5.0e−1	5.0e+0	3.4331e+0	4.9959e+0	days
	Atmosphere					
5	T diff. amp.	1.0e+6	1.0e+7	3.7548e+6	2.5839e+6	$m^2 \, s^{-1}$
6	q diff.	5.0e+4	5.0e+6	1.7447e+6	1.9337e+6	$m^2 \, s^{-1}$
7	T adv. coeff.	0.0e+0	1.0e+0	6.0357e−2	8.9163e−2	-
8	q adv. coeff.	0.0e+0	1.0e+0	1.3674e−1	1.4885e−2	-
9	Sea-ice diff.	5.0e+2	8.0e+3	6.2494e+3	7.9913e+3	$m^2 \, s^{-1}$
10	FWF adjust.	0.0e+0	2.0e+0	8.9796e−1	1.0406e+0	-
11	T diff. width	5.0e−1	2.0e+0	1.3071e+0	1.9920e+0	radians
12	T diff. slope	0.0e+0	2.5e−1	6.8597e−2	2.3644e−1	-

It is worth mentioning that it is common practice to test a parameter calibration method by an identical twin test in which an arbitrary system state is used as artificial data and the calibration method attempts to determine what parameter values were used to produce it. Indeed, the EnKF development for C-GOLDSTEIN followed this approach, with [28] showing that the EnKF was able to solve the identical twin problem in around $n \times 2000$ years, where the ensemble size n in the test was set to 54 (their Fig. 2) and [6] showing that with real data the integration cost increased to around $n \times 10000$ years (from their Fig. 4). In the case of Proximal-ACCPM, we found that if the artificial data were used as an initial state, the method was able to find the exact parameters used to extremely high accuracy in only around 100 Proximal-ACCPM iterations. With a very short integration period of two years, this gave a total integration time for estimation of the 12 parameters of less than 3000 years. In other words, Proximal-ACCPM was able to solve the identical twin test so efficiently that it was necessary to proceed directly to the case with real data to have a meaningful assessment of the method.

7.2 Model climate

As expected from the decrease in mean error, the final state $\widetilde{s}(x^*)$ of the optimisation procedure constitutes a significantly more realistic climate than the initial guess $\widetilde{s}(x^0)$. We do not discuss the model climate in detail because the final state is similar to that obtained using the EnKF procedure and discussed in detail by [6]. By way of illustration we show, in Fig. 5, the sea-surface temperature (SST) field in the final state, along with the SST difference fields between this state and the initial guess, the EnKF solution, and the data. Changes of several degrees are visible compared to the initial state, leading to broad regions of low error compared to the data. Large systematic errors remain, however, particularly in the regions of the cold upwelling pools in the eastern tropical Pacific and Atlantic and in the boundary current separation regions of the Gulf Stream and Kuroshio. These regions are challenging even for much more computationally expensive climate models. The EnKF solution has very similar SST and thus similar systematic errors, which it is reasonable to assume are inherent to the model dynamics. It is noteworthy that

the method is able to find a minimum-error state without difficulty, even when the optimal model climate is relatively far removed from the observational target.

Most intriguing is that the EnKF and Proximal-ACCPM solutions are not exactly the same. Indeed there are substantial differences in most parameters, as indicated in Table 2. According to the error estimate provided by the EnKF method the parameter values obtained using Proximal-ACCPM are, on average, around two standard deviations away from the mean obtained using the EnKF (see [6]). That the solutions are different is to be expected since, as noted above, the EnKF estimate is constrained to remain relatively close to the initial estimate. Furthermore, it was noted by [6] that certain parameters are only poorly constrained, in particular the parameter governing the behaviour of sea-ice, for which no data constraint was applied. Sea-ice diffusivity in the Proximal-ACCPM solution is very close to the imposed bound, and experience with both methods suggests that larger values are preferred. The EnKF, however, penalises solutions which are near to the bounds. Another relevant point is that [6] found certain parameters to be correlated, indicating possible redundancy in the tuned parameter set, in particular the multiple parameters governing atmospheric transport. Closer examination reveals that differences in atmospheric transport appear to physically explain the differences in the modelled climate states.

We are thus left with two significantly different sets of "optimal" parameters arising from different approaches to calibration but associated with very similar climate states. Remaining close to the original priors gives a better-posed mathematical problem, but means that the result depends on initial guesses for both the mean and the variance of the parameter distributions, rather than simply on the imposed extreme values. It must also be borne in mind, as shown by [13], that in certain regions of parameter space C-GOLDSTEIN exhibits multiple solutions for fixed parameter values, corresponding to qualitatively different steady ocean circulation states. By more devious choice of initialisation procedures, the model has been found to possess up to 12 steady solutions for fixed parameters in some regimes, mostly corresponding to qualitatively very similar states (J.Hargreaves pers. comm.). Thus it is likely that a given method could produce different solutions depending on the initial conditions and solution path. Another possibility, which cannot be ruled out, is that the optimisation procedure itself could have multiple solutions, in other words, that multiple local minima of the cost function might exist. This would be in line with the results of [14] where the Monte-Carlo optimisation, effectively a global optimisation, while admittedly undersampled, found both good and bad solutions almost throughout the range of each parameter.

Whatever the root cause, the possible existence of different optimal solutions using different methods or initial conditions indicates that, although great improvements can be obtained in the fit of model to data and thus in the objectivity of the model calibration process, it may be difficult to identify with confidence the globally optimal values for individual parameters. Climate model calibration should thus be viewed as part of a continual process of improving knowledge of model errors as a function of prior assumptions concerning model parameters.

8   Conclusions

In this paper, we have shown how oracle-based optimization can be effectively used in the calibration of intermediate complexity climate models. In a fully developed example, the 12 principal transport and mixing parameters of the C-GOLDSTEIN climate model have been estimated by using Proximal-ACCPM as the oracle-based optimization tool. In terms of goodness-of-fit, we
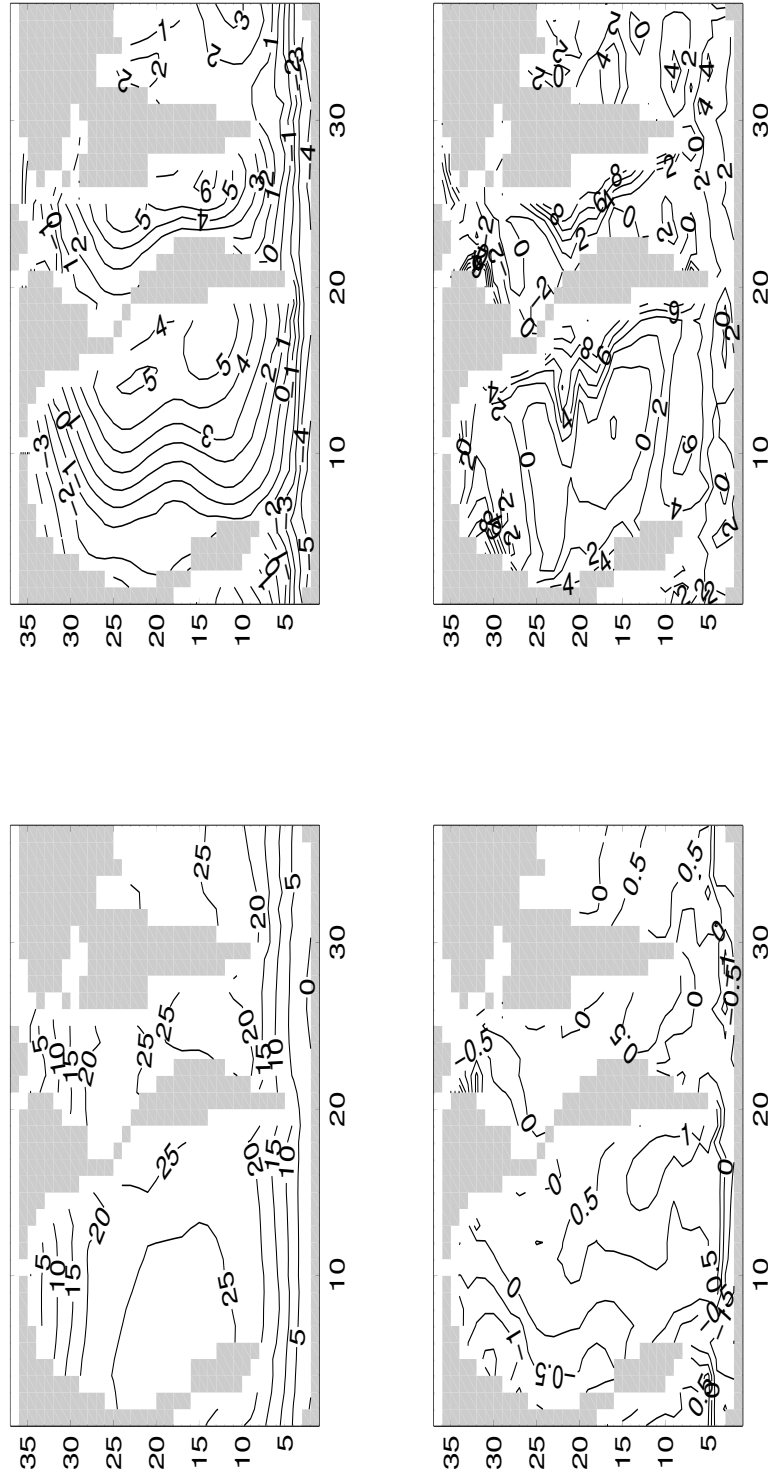
Figure 5: Final sea-surface temperature (SST) field and SST difference fields in Celcius. Upper left, the final state; upper right, final state minus initial state s^0; lower left, final state minus EnKF solution; lower right, final state minus data. Plots are in model grid coordinates.

have obtained estimates of similar quality to those obtained by an EnKF approach, but in around one tenth of the total model integration time. Nevertheless, the two approaches cannot really be compared since the EnKF approach also performs the estimate assessment. The fact that the solution found by Proximal-ACCPM was well outside the estimated error bounds provided by the EnKF warns that the results of model calibration can depend on the initial assumptions concerning model parameters. Results may also be subject to sensitivity to initial conditions, or redundancy in the process of minimizing a simple scalar error function by tuning many, related parameters in a model with large systematic errors. Overall, the result is that it may be difficult to identify with confidence the globally optimal values for individual parameters. Nevertheless, optimisation is able to produce considerable improvements in model performance and remove at least some of the subjectivity which plagues the model development process. The oracle-based optimization approach used here is highly efficient, simple to implement and generally applicable and could thus be useful in calibrating other computationally demanding models based on temporal integration (simulation), for which functional derivative information is not readily available. Whether the approach could be successfully applied to more chaotic models, such as eddy-resolving climate models, remains untested and uncertain. In [29] it is argued that pathological behaviour of even averaged statistics in such cases handicaps any derivative-based method, although the derivative-based 4DVar method is widely used for assimilation in eddying models over very short integration periods.

Our contribution has been empirical. By using a well established optimization tool, Proximal-ACCPM, we have performed a fast tuning of C-GOLDSTEIN, a model of intermediate complexity. The keys for the fast tuning have been: (1) The fast computation of the error function and approximated derivatives by exploiting the re-start procedure (warm start) in the C-GOLDSTEIN model. (2) The rapid convergence and robust behaviour, particularly in respect of non-convexity, of Proximal-ACCPM.

From the climate modelling point of view two refinements to the work described here would be highly desirable, firstly the use of an error function which incorporates information from a variety of oceanic tracers representing different timescales, and secondly developing the ability to tune two separate steady states of the model to different data sets. This would make it possible to demand that a model sucessfully reproduces more than one climate state. An obvious example would be simultaneous tuning to glacial and interglacial states.

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