27th February 2024

Re: Response to Comments of Reviewer #2- A Comprehensive Framework for Stochastic Calibration and Sensitivity Analysis of Large-Scale Groundwater Models Submission to Hydrology and Earth System Sciences

We appreciate the efforts the Reviewer has invested in our manuscript. Following is an itemized list of the comments together with our response to each. Comments are listed in black italic font and our responses in blue font. Proposed revisions to the original text are in red fonts.

Sincerely,

Andrea Manzoni, Giovanni Michele Porta, Laura Guadagnini, Alberto Guadagnini, Monica Riva

This paper presents a pioneering framework designed to model large-scale groundwater systems using a comprehensive three-dimensional approach. This approach not only accounts for the dynamics of river-aquifer interaction but also integrates three-dimensional spatial distributions of geo-materials. Notably, the framework excels in achieving a delicate equilibrium between the requisite simplification essential for large-scale groundwater models and the anticipated outcomes. Of particular significance is the utilization of a multi-objective optimization approach for model calibration and sensitivity analysis.

We thank the Reviewer for the insightful review and positive feedback on our paper. We appreciate that you found our framework to be pioneering in its approach to modeling large-scale groundwater systems. The recognition of the value of our comprehensive three-dimensional approach, which considers both river-aquifer interaction dynamics and the spatial distributions of geo-materials, reinforces our determination in future research efforts in this context. We particularly appreciate the acknowledgment of the delicate equilibrium we sought to achieve between simplification and outcome accuracy in large-scale groundwater modeling. Striking this balance is indeed a key focus of our framework of analysis and modeling. We sincerely appreciate the time invested by the reviewer on our work and look forward to any further insights or suggestions.

From a general standpoint, I have two major concerns before recommending the paper publication:
Comment #1:

*This study, is build upon the substantial groundwork laid by Manzoni et al. (2023), a fact that merits explicit acknowledgment in both the introduction and the abstract. Indeed, in my opinion, the contributions made in Manzoni et al. (2023) represent a cornerstone of the framework presented herein, serving as more than just a dataset but rather as a fundamental component upon which this work is built.*

Answer #1:

We appreciate your recognition of the substantial groundwork laid by Manzoni et al. (2023), which indeed serves as a fundamental component of our framework. We agree that this element deserves explicit acknowledgment in both the introduction and the abstract, and we will revise these sections accordingly. Prompted by the Reviewer, we will cite Manzoni et al. (2023) more prominently throughout the paper (e.g., answer to comment #3 of Reviewer #1), highlighting their contributions to the field and how our work builds upon them. The revised manuscript will include the following paragraphs.

Into the Abstract:

“We address the challenges posed by the characterization of the heterogeneous spatial distribution of subsurface attributes across large-scale three-dimensional domains upon incorporating a recent probabilistic hydrogeological reconstruction specific to the study case.”

Into the introduction:

“In some cases, system properties are assumed to be constant along the vertical direction (e.g., Maxwell et al., 2015; Shrestha et al., 2014; Soltani et al., 2022) without taking into account the three-dimensional nature of the spatial heterogeneity of the subsurface system. In this sense, parameter values are typically inferred from literature information (Naz et al., 2023; Maxwell et al., 2015), thus possibly introducing large margins of uncertainty that are seldom quantifiable. The work of Manzoni et al. (2023) addresses these challenges by proposing a machine-learning-based methodology for delineating the spatial distribution of geomaterials across large-scale three-dimensional subsurface systems. These authors showcase their approach upon focusing on the Po River Basin in northern Italy. Their work provides a comprehensive dataset comprising lithostratigraphic data from various sources and offers a robust framework for quantifying prediction uncertainty at each spatial location within the reconstructed domain. Hence, our study rests on the findings of Manzoni et al. (2023). In these sense, the latter serve as more than simply a dataset but as a critical component upon which we build our groundwater flow model calibration.

…”

The approach involves the development of a groundwater model that includes a probabilistic three-dimensional hydrogeological reconstruction of the investigated area. As stated above, we do so upon integrating the result illustrated by Manzoni et al. (2023). Specifically, we leverage on their probabilistic three-dimensional hydrogeological reconstruction, which enables us to infer the spatial distribution of geological properties at a scale that was previously unattainable. By incorporating this
advanced hydrogeological reconstruction into our workflow, we address key challenges posed by uncertainties that are inherent to large-scale groundwater systems.”

Comment #2:

The aspects presented in lines 59-61 may not inherently appear novel 'per se'. The authors should thus better emphasize the unique contributions and novelties of their work to distinguish it from existing literature.

Answer #2:

Prompted by the Reviewer, we will explicitly state the novel aspect of our approach right after lines 59-61 of the original manuscript. This will involve clarifying how our work builds upon (or departs from) existing research in a way that contributes to yield new insights or solutions. We will reassess the wording and framing of the paragraph pointed out by the Reviewer to ensure that it effectively communicates the original features of our study. The revised text now reads:

“Here, we introduce and test a methodological approach for stochastic model calibration tailored to large-scale scenarios (exceeding 10,000 km²). Our proposed methodology combines a suite of tools that have not been previously employed to address groundwater modeling at such a vast scale and with such level of system complexity. This includes (a) modeling the dynamics of groundwater movement across a three-dimensional setting, (b) embedding and analyzing in details interactions between rivers and aquifers, (c) relying on a probabilistic reconstruction of geological material distributions and attributes, (d) resting on multi-objective optimization techniques for stochastic calibration of large-scale groundwater models, and (e) performing a detailed informed global sensitivity analysis to assess the degree of spatial variability of the relative importance of uncertain model parameters therein. Through incorporation of these tools, our methodological and operational workflow yields a calibrated model that enhances understanding of aquifer dynamics from a holistic perspective and reveals insights into the spatial pattern of the sensitivity of model outputs to model parameters. Results associated with the latter element can be employed to inform future data acquisition efforts to improve model parameterization and hydraulic head estimates and emphasize the need to balance model complexity with simplifications that might be required to tackle large-scale groundwater modeling.”

Other specific comments:

Comment #3:

In light of Manzoni et al. (2023), the statement highlighting the limitations of data-driven models due to constraints in the quantity and quality of available training data, particularly in large-scale scenarios where data accessibility across the entire domain might be limited, warrants revision. Specifically, it should be contextualized to reflect insights gleaned from Manzoni et al. (2023) and potentially revised to underscore the advancements or strategies proposed in this study to address such challenges.
Answer #3:

We appreciate the Reviewer's insightful comment. The constraint on data availability currently pertains specifically to groundwater flow and pressure data, at least in the area analyzed. As outlined in Section 3.3.1 (Data curation), our study relies on a limited dataset comprising 286 wells where data can be employed for groundwater model calibration. The study by Manzoni et al. (2023) is focused on the reconstruction of the spatial distribution of geomaterials and leverages on a robust dataset associated with more than 50,000 wells. This yields more than 2 million data points associated with geological information and adequately supports the application of data-driven machine learning approaches for hydrogeological reconstruction. It is also noted that localized areas exhibiting high uncertainty in the geological material distribution due to limited data availability primarily lie outside the lateral boundary of the modeled groundwater system (see also Manzoni et al. (2023)). The revised manuscript will include the following two modifications and additions in Introduction and Section 3.2., respectively.

“It is noted that data-driven models are heavily constrained by the quantity and quality of available training data. In this context, groundwater flow and pressure data may not be as readily accessible as, for example, lithostratigraphic data (see e.g., Manzoni et al., 2023) across the entire domain, especially when considering large-scale scenarios.

…”

Notably, the highest uncertainties in the hydrostratigraphic reconstruction model are found beyond the lateral boundaries of the groundwater system, where only a limited number of investigations is available.”

Comment #4:

The clarity of Equation “\( Q_s = r_q R_s S_s \)” is ambiguous. Assuming my interpretation is correct, where the subscript \( s \) represents the \( s \)-th subbasin, further clarification from the author is needed regarding whether the efficiency term is constant across time or space. Additionally, a more detailed discussion on the assumption of the correction coefficient, \( r_q \), being constant for all subbasins would enhance understanding. This could include explanations of the rationale behind this assumption, any potential implications or limitations, and how it aligns with existing literature or empirical evidence.

Answer #4:

Prompted also by a comment of Reviewer #1, the expression "\( Q_s = r_q R_s S_s \)" is now addressed as a standalone equation within the manuscript. This adjustment enables us to provide a comprehensive elucidation of the underlying assumptions guiding its formulation. Introducing individual \( r_q \) values for each sub-basin would increase the level of complexity of the parameterization process, potentially resulting in model over-parameterization and subsequent overfitting of data. Notably, Figure 7 documents that simulated hydraulic heads demonstrate increased sensitivity to \( r_q \) near the lateral boundaries of the domain. In this context, fine-tuning \( r_q \) values for each sub-basin could lead to overfitting. We will implement these considerations in Section 3.2 of the revised manuscript. The revised text now reads:
Making use of the results of Sect. 3.1, we evaluate within each of these sub-basins the average (in time) amount of water that infiltrates within a day as

\[ Q_s = r_q R'_s S_s, \]  

where \( R'_s \) [L/T] is the (space-time averaged) recharge rate evaluated for the \( s \)-th sub-basin (with ground surface area of \( S_s \)) during the temporal window spanning the years 2013-2019. To account for possible exfiltration of infiltrated water or infiltration of water due to surface-groundwater interaction (e.g., river water infiltration), we also introduce a correction coefficient, \( r_q \). The latter is set at a constant value for all sub-basins to avoid model overparameterization and is estimated through model calibration, as detailed in Sect. 3.3.

Comment #5:

The description of the domestic water flux associated with groundwater resource utilization lacks the necessary details for reproducibility and applicability in other areas. To enhance the transparency and replicability of the work, it is suggested that the authors provide additional information regarding the data utilized, including its sources and any assumptions or hypotheses underlying its selection or interpretation. This could involve detailing the methodology for acquiring the total volumetric flow rate associated with groundwater extractions of drinking water within a municipality, as well as specifying the criteria used to define the surface area covered by the municipality. By providing this supplementary information, the study’s findings can be better contextualized and applied to different geographical regions or scenarios.

Answer #5:

In response to the Reviewer’s suggestions, we will detail the methodology used to acquire the total volumetric flow rate associated with groundwater extractions for drinking water within each municipality. Furthermore, we will specify the criteria used to define the surface area covered by each municipality, ensuring clarity and consistency in our spatial delineation. In this context, we will modify the text in the designated section as follows.

“To estimate the volumetric flow rate for domestic use, we rely on the public water supply data provided by the Italian National Institute of Statistics (ISTAT, 2020). This dataset contains values of flow rates (in m³/year) employed for domestic purposes for each municipal administrative area and the share of domestic water associated with groundwater resources. Such data are available for the years 2012, 2015, 2018, and 2020. We then evaluate the average flow rate for each municipality on these bases. For a given municipality, domestic water fluxes associated with the use of groundwater resources is assessed upon evaluating the ratio of the total volumetric flow rate associated with groundwater extractions for drinking water to the surface area covered by the municipality itself (OpenStreetMap, 2021). Volumetric flow rates employed in the model are then obtained by multiplying the portion of the municipality area within the modeled domain by the domestic water flux. Due to the lack of comprehensive information regarding the location of extraction wells, we consider such a water flow rate as a distributed sink term located within the deepest layer of the simulation domain beneath each associated municipality. This assumption is grounded on the notion that drinking water wells are typically engineered to extract water from locations that are protected from potential contaminants that may infiltrate and pollute shallower regions of subsurface water bodies.”
References

Comment #6:
The section pertaining to multi-objective calibration appears to lack clarity and would benefit from a more precise formulation of the mathematical framework. It is recommended to clearly define the two objective functions, delineate the independent variables, and specify any constraints involved in the optimization process. Providing explicit details about the mathematical formulation will enhance understanding and facilitate the replication of the calibration methodology.

Answer #6:
In response to this suggestions, we will revise the section to explicitly define the two objective functions separately. We move the algorithm description from Appendix A into the text and improve the algorithm description upon focusing on mathematical formulation details to assist replicability of the calibration methodology (see also answer to comment #7). To further improve the description and the replicability of the implemented algorithm, we also plan to add an image containing the pseudocode. The revised manuscript now reads:

“Model parameters are estimated through a multi-objective optimization approach. The latter is tied to the joint minimization of two objective functions formulated as

\[ f_{N_{hb}} = \sqrt{\frac{\sum_{l=1}^{N_{hb}} (\hat{h}_l - h_l)^2}{N_{hb}}} \]  

(6)

and

\[ f_{N_{hr}} = \sqrt{\frac{\sum_{l=1}^{N_{hr}} (\hat{h}_l - h_l)^2}{N_{hr}}} \]  

(7)

where \( \hat{h}_l \) and \( h_l \) denote observed and estimated hydraulic head at well \( l \), respectively. Estimation of permeability of each geomaterial (i.e., \( k_c \) in Eq. 3) and of the correction coefficient (i.e., \( r_q \) in Eq. 4) entails minimizing Eq. (6) (considering all available hydraulic head data, \( N_{hb} \)). To estimate the specific conductance of the riverbeds, \( \alpha_r \) (with \( r = 1, \ldots, 20 \)), we minimize Eq. (7) with \( N_{hr} < N_{hb} \), where \( N_{hr} \) is the number of wells located within a maximum distance of 5 km from a river (see orange dots in Fig. 1). Including this constraint on the distance between a river and observation wells enables us to refine the estimation of \( \alpha_r \) by considering only hydraulic head observations that are significantly impacted by the interconnection between the groundwater system and the rivers. Note that minimization of Eq. (6) and (7) is tantamount to relying on a Maximum Likelihood (ML) estimation approach assuming that measurement errors of hydraulic head are not correlated and can be described through a Gaussian distribution (Carrera and Neuman, 1986).“

...
The implemented algorithm is designed to address global optimization problems through alternate evolution of candidate solutions between the two different species. The algorithm uses mutation, crossover, and selection strategies to enhance the quality of solutions as detailed in the following. First, we introduce the populations of candidate solutions. For each of the two species (where ‘sp’ takes the values of one or two, for species associated with Eq. (6) or (7), respectively), we consider a set of $N_s$ candidate solutions (or members), denoted as $S_{sp} = [s_{sp,1}, ..., s_{sp,m}, ..., s_{sp,N_s}]$. Following Storn and Price (1997), we set $N_s = 15 \times N_p$, $N_p$ being the number of parameters (i.e., $N_p = 7$ or 20 for Eq. 6 or Eq. 7, respectively). Initial candidate solutions are defined by randomly selecting parameter values from a parameter space whose extent is designed to encompass a broad range of possible solutions.

Members of the populations are combined and mutated to calculate the next generations of candidate solutions as follows. We start by computing a mutated vector for each $m$-th candidate solution of a species associated with the $k$-th iteration of the optimization algorithm (or generation) as:

$$\hat{s}_{sp,m}^k = s_{sp,m}^k + F \left( s_{sp,a}^k - s_{sp,b}^k \right),$$

Here, $F$ represents an algorithm parameter (termed differential weight) that is set equal to 0.5 and $s_{sp,a}^k$ and $s_{sp,b}^k$ (with $a \neq b \neq m$) correspond to two (randomly selected) members of the population. We then combine parameters of $\hat{s}_{sp,m}^k$ and $s_{sp,m}^k$ to determine the trial vector $\tilde{s}_{sp,m}^k$: if a parameter of $\hat{s}_{sp,m}^k$ is selected for mutation, its value is taken from $\hat{s}_{sp,m}^k$; otherwise, it is taken from $s_{sp,m}^k$. We randomly choose the parameters of $s_{sp,m}^k$ that will undergo mutation among the parameters associated with the $sp$ species, with a probability of parameter mutation set to 0.5. We finally select the $m$-th candidate solution of the $(k+1)$-th generation, $s_{sp,m}^{k+1}$, by comparing the trial member, $\tilde{s}_{sp,m}^k$, and the $m$-th population member from the $k$-th generation, $s_{sp,m}^k$, based on the following condition:

$$s_{sp,m}^{k+1} = \begin{cases} \tilde{s}_{sp,m}^k, & \text{if } f_N(\tilde{s}_{sp,m}^k) < f_N(s_{sp,m}^k) \\ s_{sp,m}^k, & \text{if } f_N(\tilde{s}_{sp,m}^k) \geq f_N(s_{sp,m}^k) \end{cases} \quad \text{with } f_N = f_{Nh_f} \text{ or } f_{Nh_r}. \quad (9)$$

The algorithm steps can be summarized as follows at a given iteration $k$:

1. Calculate a new generation $(k+1)$ of the first species using Eqs (8)-(9) with $f_N = f_{Nh_f}$, while keeping the parameters of the second species fixed;
2. Transfer the parameter set with the best performance, $s_{1, best}^{k+1}$, among the members of $s_{1,m}^{k+1}$ to the second species;
3. Maintain the parameters of the first species as fixed while calculating $s_{2,m}^{k+1}$ (the next generation of the second species), thus repeating step 1 for the second species with $sp = 2$ and Eq. (7);
4. Pass back to the first species the parameter set of the member in the second species with the best objective function value, $s_{2, best}^{k+1}$;
5. Repeat steps 1 to 4 until a stopping criterion is met.

The patience stopping criterion is here employed for both objective functions, i.e., the algorithm stops if no improvement in performance over 80 consecutive iterations (or epochs) is detected. Figure 3 illustrates the Pseudocode of the algorithm.
Begin
Initialize $S_1 = [s_{1,1}, \ldots, s_{1,m}, \ldots, s_{1,Ns_1}]$ and $S_2 = [s_{2,1}, \ldots, s_{2,m}, \ldots, s_{2,Ns_2}]$.
Evaluate the members of $S_1$ using Eq. (6).
Evaluate the members of $S_2$ using Eq. (7).
While stopping criteria are not met for both the species:
   For each $m$-th member of $S_1$
      Create $\tilde{s}^{k \_m}$ by applying mutation and crossover.
      Evaluate $\tilde{s}^{k \_m}$ using Eq. (6).
      Select $s^{k+1 \_m}$ according to Eq. (9).
      Select $s^{k+1 \_best}$
   EndFor
   Fix the parameters associated with Eq. (6) equal to $s^{k+1 \_best}$.
   For each $m$-th member of $S_2$
      Create $\tilde{s}^{k \_m}$ by applying mutation and crossover.
      Evaluate $\tilde{s}^{k \_m}$ using Eq. (7).
      Select $s^{k+1 \_m}$ according to Eq. (9).
      Select $s^{k+1 \_best}$
   EndFor
   Fix the parameters associated with Eq. (7) equal to $s^{k+1 \_best}$.
   k++
EndWhile
Return $s^{k+1 \_best}$ and $s^{k+1 \_best}$.
End

Figure 3: Pseudocode of the employed algorithm.

Comment #7:

The authors should provide further clarification regarding the statement "We note that CCDE does not require defining a single weighted multi-objective function, as otherwise required by the standard DE." It would be beneficial to elaborate on the distinction between the adopted algorithm (CCDE) and the standard NSGA-II algorithm. For example, the NSGA-II algorithm does not inherently require a weighted multi-objective function either. Algorithms such as NSGA-II typically operate based on the concept of dominance and the Pareto front without necessitating explicit weight assignment during the optimization process. Therefore, expanding on the characteristics of CCDE and how it differs from conventional multi-objective optimization algorithms like NSGA-II would provide valuable insights. Furthermore, it appears that the original paper by Storn and Price (1997) primarily focuses on single-objective optimization, similar to the work by Trunfio in 2015. Given that the current study deals with non-contrast objective functions, it may explain the absence of weight utilization. However, providing additional details on the rationale behind the choice of CCDE and its suitability for handling the specific characteristics of the optimization problem in this context would enhance understanding.
Answer #7:

As the Reviewer correctly points out, the Coevolutionary Differential Evolution (CCDE) proposed by Trunfio (2015) is designed for single-objective optimization. In our case, the coevolutionary algorithm is adapted to handle two objective functions. Specifically, the two evolving species are associated with two different objective functions (i.e., Eq. 6 and Eq. 7 in the revised manuscript). In this context, we revise the manuscript according to our answer to comment #6 to guarantee replicability of the methodology.

We plan to revise the sentence highlighted by the Reviewer to clarify that we have implemented a modified version of the coevolutionary differential evolution algorithm. We also intend to amend the original manuscript to underscore the main differences and similarities between the algorithm we used and the NSGA II as follows.

“The two objective functions to minimize are closely interconnected. We implement an enhanced variant of the Differential Evolution (DE) optimization method (Storn and Price, 1997) to effectively minimize both objective functions simultaneously. Here, we rest on a modified version of the Cooperative Coevolutionary Differential Evolution (CCDE) optimization algorithm proposed by Trunfio (2015) tuned to our problem, which is an adaptation of the standard DE algorithm to the theory of Coevolutionary Algorithms (CAs). The implemented algorithm does not require defining a single weighted multi-objective function, as otherwise required by standard DE and standard CCDE. Thus, our approach eliminates the non-trivial task of determining the appropriate (relative) weights between each of the terms that constitute the multi-objective function (e.g., Dell’Oca et al., 2023). Resorting to a modified CCDE algorithm enables us to balance between simplicity and the efficiency documented for CAs when dealing with multi-objective fitness functions (Khan et al., 2022).

As nature-inspired optimization techniques, CAs draw upon principles of biological coevolution, where optimization problems are linked to coevolving species (Dagdia and Mirchev, 2020). CAs share similarities with Evolutionary algorithms, as their sampling mechanisms and dynamics are inspired by Darwin’s Theory of Evolution. Just as species evolve based on their fitness to survive and reproduce within an environment, solutions within a search space evolve to achieve the minimum of an objective function (Simoncini and Zhang, 2019). Additionally, the coevolution principle considers that a change in one species can trigger changes in related species, thus leading to adaptive changes in each species (Khan et al., 2022). In this context, Eq.s (6) and (7) represent optimization functions for two coevolving species. These are then optimized through the modified CCDE. Our algorithm differs from CCDE (Trunfio, 2015) primarily in the way we define the dimensions of the two species. Instead of employing random or dynamic grouping strategies (Zhenyu et al., 2008; Trunfio, 2015), we opt for a supervised grouping strategy linking one of the model parameters (i.e., riverbed conductance, \( \alpha_r \)) to one species and the remaining parameters to the other species.

We choose a modified version of Coevolutionary Differential Evolution (CCDE) over the widely used NSGA II (or its variant CC-NSGA-II) for our algorithm. Both these algorithms use a divide-and-conquer strategy and are effective for high dimensional optimization. However, while NSGA II relies on a genetic algorithm, our algorithm utilizes Differential Evolution (DE). According to Tusar and Filipic (2007), DE-based algorithms outperform GA-based algorithms in multi-objective optimization.
due to a more efficient exploration of the parameter space. This element is particularly critical when optimal solutions lie on parameter bounds or amidst many local optima.

Additionally, our implemented algorithm does not explicitly optimize a front, which is otherwise a central concept in NSGA-II. Instead, it focuses on optimizing individual objective function values without introducing a dominance concept considering both objectives. This approach leads to a single set of optimized parameters, thus simplifying the optimization process through a balance of the contribution of both objective functions.”

References


Comment #8:

It is suggested that the authors include a figure illustrating the framework chain, depicting the data inputs required as well as the expected outcomes. This visual representation will aid in comprehending the workflow of the methodology and provide a clear overview of the research process. Additionally, the figure can serve as a useful reference for readers to understand how various components of the framework interact and contribute to the overall analysis.

Answer #8:

Prompted by the Reviewer, we will include the following new figure illustrating the framework chain to enhance clarity.

![Conceptual workflow for stochastic calibration and sensitivity analysis of large-scale groundwater models.](image-url)

Figure 1: Conceptual workflow for stochastic calibration and sensitivity analysis of large-scale groundwater models.