Author Response to RC1: “Computationally efficient subglacial drainage modelling using Gaussian Process emulators: GlaDS-GP v1.0”

Reviewer: Vincent Verjans

Tim Hill, Derek Bingham, Gwenn E. Flowers, Matthew J. Hoffman

Reviewer comments are in black and we provide our responses in blue.

This study develops a Gaussian Process (GP) emulator to emulate output from the subglacial hydrology model GlaDS (Werder et al., 2013). In particular, the GP is trained to reproduce the sensitivity of flotation fraction output to 8 different GlaDS parameters. A principal component truncation is performed to reduce the dimensionality of the outputs to be emulated. Training is performed on an idealized glacier configuration, with a pre-specified melt input forcing. The performance of the emulator is then evaluated on 100 test combinations of GlaDS parameters, unseen during the emulator training.

This study contributes positively to efforts towards computationally efficient solutions to simulate subglacial hydrology. It also offers a promising tool to evaluate parametric uncertainty of subglacial hydrology models. This latter aspect is important, since subglacial hydrology models are heavily parameterized, with very few physical constraints on parameter values. I value positively the technical approach used for the emulator development. On the idealized configuration tested here, the emulator shows a good performance on non-training data samples. The manuscript is clearly structured and well-written. I have nonetheless a concern regarding the impact of the study. The authors have developed a subglacial hydrology emulator, but the real scientific value of this lies in the implications for areas where subglacial hydrology plays a role, many of which are provided as motivations in the introduction. As presented, both the emulator performance and the potential for uncertainty quantification are hard to interpret, because no application of the emulator is demonstrated. I detail this concern in my Major comment below, and I emphasize that this lack of impact (1) is my personal opinion, and it is the editor who decides which impact is expected from studies published in Geoscientific Model Development, and (2) does not influence my positive opinion about the quality of the work performed by the authors, but only on what more could be done. My review further includes a Minor comment regarding the quantitative evaluation of the emulator, and Technical comments aiming to improve the structure and clarity of the manuscript. Line numbers in this review correspond to the preprint manuscript.

Thank you for the detailed review and sharing your expertise in this area. We appreciate your suggestions to improve the manuscript and plan to implement them in the revised version. We have responded to your comments individually below.

Major comment: Impact

As mentioned in my introduction, emulation and uncertainty quantification of subglacial hydrology by themselves are not of great scientific interest. It is really the implications of subglacial hydrology for different fields, primarily ice flow modeling but also others listed in the introduction, that make it a critical research topic. However, none of these implications is explored here. As such, I feel like the prediction performance and the potential for uncertainty quantification from the GP emulator are not very meaningful as presented.

I note that GlaDS has been run with the Ice-sheet and Sea-level System Model (ISSM, Larour et al., 2012). As such, it should not be a big step to compute ice flow simulations (1) using the GlaDS output and (2) using the emulator output in order to evaluate the implications of emulator performance on modeled ice flow. Furthermore, it would be very interesting to see differences in modeled ice flow across the range of GlaDS parameters investigated in this study. This would really demonstrate the benefits of uncertainty quantification of subglacial hydrology when it comes to modeling ice flow velocities. Even though this study focuses on a single idealized glacier and melt forcing configuration, such ice sheet model experiments would be a great contribution to constraining ice flow uncertainty caused by subglacial hydrology.

If the authors are concerned about the length of the manuscript if such experiments are included, I would recommend reconsidering the inclusion of the simulations of scalar quantities (f_Q, T_s, and L_c). In my view, these experiments are not of great relevance, as I do not see which research area would benefit from predictions and uncertainty quantification of these variables. Again, I repeat here that the decision of sufficient impact from this study for publication in Geoscientific Model Development is ultimately a decision of the editor. I express here my personal opinion. And I emphasize that the work presented in this manuscript is of good quality, with only a single Minor comment and some Technical comments that I provide below.

Thank you for suggesting ways to make the work more interesting to a broader audience. However, we disagree with the statement that subglacial drainage modelling by itself is unimportant and uninteresting. For example, Ehrenfeucht et al. (2024) recently pushed physics-based subglacial drainage modelling forward by producing full-Antarctic GlaDS runs. That this work was published in GRL suggests community interest in subglacial drainage modelling. Moreover, recent work towards understanding the physics of subglacial drainage models (e.g., Sommers et al., 2023; Warburton et al., 2024), and constructing models with approximate physics in order to improve computational scaling (Kazmierczak et al., 2024) is evidence that model developments are a community priority. These latter works have highlighted open questions about drainage models that warrant attention separately from their application to ice-sheet modelling.

The suggestion to include an ice-flow component in the current work is an interesting idea that we have considered throughout the process of the larger project that this paper is one part of. We have not done so here because we believe that including an appropriately detailed and nuanced ice-flow application would be out of scope for this model description paper. Given uncertainty arising from the choice of a sliding law, the representation of basal drag would be a nontrivial addition. Moreover, forcing an ice-sheet model one-way with emulated effective pressure fields would miss important two-way hydrology–dynamics feedbacks (e.g., Hoffman et al., 2014), and running two-way coupled simulations remains non-trivial even with ISSM-GlaDS. It is also not clear how interesting the ice-flow application would be for the synthetic geometry that we have used. The uncertainty-aware emulation methods that we have used can be one part of accepting and quantifying these uncertainties, but this is out of the scope of the current work. We have summarized this discussion in an expanded Section 6.6 (Applications and Considerations).

Finally, we would like to highlight a recent preprint where we explore calibrating the subglacial drainage model with borehole water pressure data (https://doi.org/10.31223/X5GQ68). We had intended to include an ice-flow component in this work to allow for calibration with both borehole water pressure and seasonal surface velocities. However, this preprint identifies serious shortcomings in the model relative to the data, indicating that further work is needed on the subglacial drainage models themselves before their potential for ice-sheet modelling can be fully realized.

Minor comment: Quantitative evaluation

The title of Section 6.1 is "What is the fidelity of the subglacial drainage model emulator?". In my view, this question has not been evaluated thoroughly enough. I think that simply adding a table with important evaluation metrics would be sufficient to address this concern. Evaluation metrics could be averaged spatio-temporally as well as across the 100 test simulations. It would be insightful to provide 5th, 50th, and 95th percentiles of RMSE, MAPE, coefficient of determination (R^2), and bias across the 100 test simulations, where these metrics are time- and spatially-averaged. In addition, it would be nice to add the same metrics but (i) for the upper and lower 30 km parts of the domain separately, and (ii) for the DJF and JJA months separately. Such evaluation metrics would give the reader a better and more quantitative appreciation of the performance of the GP emulator. Finally, for each of these metrics, I recommend also providing between parentheses the same metric but computed on the training data. This would be insightful to evaluate the potential degradation of the GP emulator performance when used on inputs unseen during training.

Thank you for the suggestion to add the table and include the coefficient of determination (R^2). We have added the suggested table (copied below), that provides mean and 5th and 95th percentiles for each suggested statistic, to Section 4.2.2 "Model evaluation" and have referenced this table in Section 4.2.2 and Section 6.1. Since the GP interpolates the training data (c.f., neural nets), we fear that providing those statistics would be misleading, so we provide only statistics on the test data.

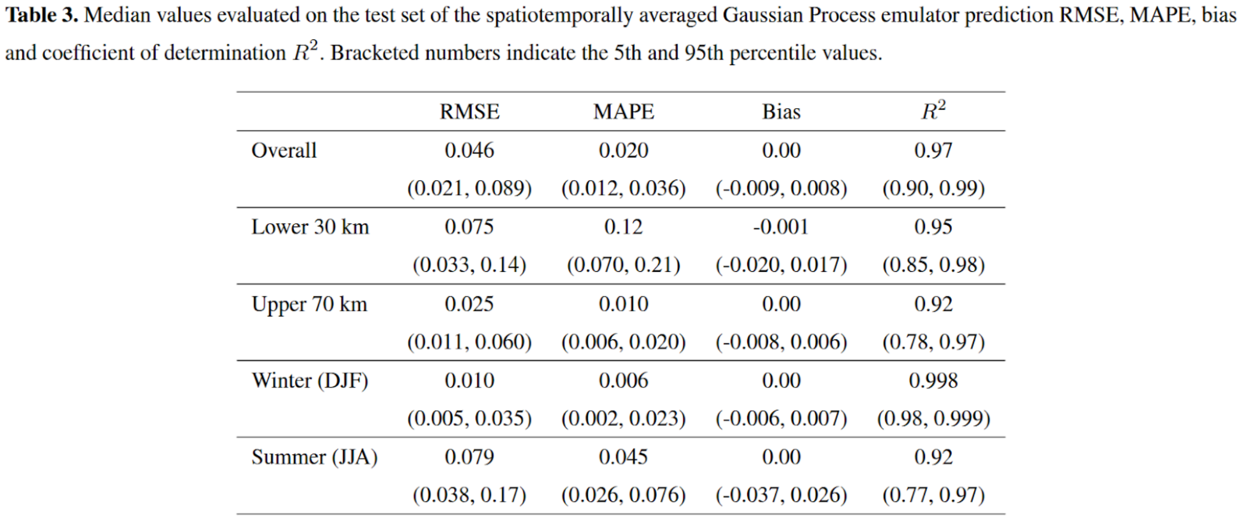


Table 3. Median values evaluated on the test set of the spatiotemporally averaged Gaussian Process emulator prediction RMSE, MAPE, bias and coefficient of determination R^2. Bracketed numbers indicate the 5th and 95th percentile values.

	RMSE	MAPE	Bias	R^2
Overall	0.046 (0.021, 0.089)	0.020 (0.012, 0.036)	0.00 (-0.009, 0.008)	0.97 (0.90, 0.99)
Lower 30 km	0.075 (0.033, 0.14)	0.12 (0.070, 0.21)	-0.001 (-0.020, 0.017)	0.95 (0.85, 0.98)
Upper 70 km	0.025 (0.011, 0.060)	0.010 (0.006, 0.020)	0.00 (-0.008, 0.006)	0.92 (0.78, 0.97)
Winter (DJF)	0.010 (0.005, 0.035)	0.006 (0.002, 0.023)	0.00 (-0.006, 0.007)	0.998 (0.98, 0.999)
Summer (JJA)	0.079 (0.038, 0.17)	0.045 (0.026, 0.076)	0.00 (-0.037, 0.026)	0.92 (0.77, 0.97)

Technical comments

- General (1): The authors make an excessive use of parentheses throughout the text. In my view, parentheses should only be used to provide additional non-essential details in the text. I recommend that the authors clean up their parentheses by making more sentence separations instead of overloading single sentences.

  We have simplified the language throughout where it has been appropriate and there are now fewer parentheses than the original manuscript. In many cases, especially in Section 2.2 (Gaussian Process model), we retain parentheses to provide in-line definitions or examples of technical language to ensure that non-experts can follow the text.

- General (2): Throughout the manuscript, the authors use both the terms “inputs” and “parameters” to refer to the same notion: the parameters of GlaDS passed to the emulators. To avoid any confusion, a single term should be used consistently in the entire manuscript.

  Thank you for highlighting that these two terms were used interchangeably for the same object. As suggested, we have changed most instances of “inputs” to “parameters” or “GlaDS parameters”. We have retained a few instances of “inputs” since it has sometimes been useful to speak about “inputs to the emulator” more abstractly than by referring to the GlaDS parameter values, particularly in Section 2 where we provide a high-level overview of the GP emulator. We have acknowledged this by stating that “Following the vocabulary of Higdon et al. (2008) and Verjans et al. (2024), these GlaDS model parameters are called the inputs to the emulator”. We have moved this statement into the beginning of Section 2 where we introduced the concept of a GP emulator and before the first instance of “inputs”. Whenever “inputs” is now used, we have clarified that we mean “emulator inputs” or “inputs to the emulator” to indicate that we are talking about the GP methodology more abstractly.

L5: Replace “construct robust” by evaluate uncertainty in.
Done.

L6: uncertainty quantification.
If we understand the reviewer correctly, this suggestion is to replace “uncertainty” with “uncertainty quantification” in the sentence: “Here, we develop Gaussian Process (GP) emulators that make fast predictions **accompanied by uncertainty [quantification]** of subglacial drainage model outputs”. What we mean to say here is that predictions have associated uncertainty, so we have revised this sentence to read: “Here, we develop Gaussian Process (GP) emulators that make fast predictions **with associated uncertainty** of subglacial drainage model outputs”.

L14: “of the water pressure variance”: it is unclear if this refers to spatial variance, temporal variance, and/or variance across the samples of the parameter space.
Thank you for highlighting this point, we mean variance as parameters are changed. We have revised this statement to: “[...] 90% of the variance in modelled water pressure in response to parameter changes”

L15: I believe that the mention to observational data is misused here, as no observational data is integrated in this study.
We have included a reference to integrating observational data to highlight this as an extension of the methods that we describe in this work: “The GP emulator approach described here is well-suited to integrate observational data with models to make calibrated, credible predictions of subglacial drainage”. As part of another reviewer’s comments, we have added a paragraph to Section 6.6 Applications and considerations that outlines how this work could be extended to calibrate model parameters. We hope that this discussion that we have added helps to provide additional details and context for this suggestion of related future work.

L25: “well-established”: I understand what the authors mean here. However, this wording is misleading, because although there is consensus about the existence of an influence of subglacial hydrology on ice flow, this influence remains highly uncertain.
This is a good suggestion, we have rephrased this statement to: “Most commonly, studies of subglacial hydrology are motivated by the influence on ice-flow velocities of glaciers …”

L26: Replace flow by sliding.
We are trying to be careful here to not explicitly imply hard-bed sliding, including also the possibility of effective pressure-dependent sediment deformation. We have changed the two instances of “basal flow” to “basal slip”, a more common catch-all term to encompass both of these processes (e.g., Cuffey & Paterson, 2010; Zoet & Iverson).

L31-36: This sentence is too long, and I do not know what “which” (L36) refers to.
We agree and have removed “, which guides the selection of model physics” since it is not necessary to make our point. Each set of references is already directly associated with a specific contribution to our understanding of subglacial hydrology.

L36: Replace large by high-dimensional.
Done.

L52: Typo: “GP emulators we develop”.
We have corrected this to “The Gaussian Process emulators we develop take subglacial drainage model parameters as their inputs”

L53: I suggest this definition for flotation fraction: ratio of water pressure to ice-overburden pressure.
Thank you, we will take this definition as it is more clear.

L55: Please explain here the meaning of “global sensitivity indices”.
We have changed “to” to “that” in the following sentence to provide a definition of the global sensitivity indices: “we compute variance-based global sensitivity indices **~~to~~ that** precisely determine the combinations of parameters that most strongly control modelled subglacial hydrology”

L63: If possible, please use another word than “emerging”.

This has been changed to “[...], with the channel ~~network emerging from~~ **radius determined by** the balance between creep closure of ice and opening by melt”

L69: Please provide units of variables.
We have added units for hydraulic potential (Pa), sheet thickness (m) and channel area (m^2)

Eq. (1): Although obvious, please define g.
Added to the description of Eq. (1), g is gravitational acceleration (Table 2).

L77: “ each of these quantities defines a two-dimensional, time-varying field”: this is confusing because I believe that both zb and pi are not time-varying.
Thanks for pointing this out, we have clarified that “**ϕ**, N and fw are two-dimensional, time-varying fields”, since zb and pi are not time-varying.

L83: Please specify: For details about GPs
Following another reviewer's suggestion, we have integrated the content from Appendix B into the main text. We have revised this reference to more precisely point to the appropriate material: “For background on Gaussian Processes see Jones et al. (1998) and Rasmussen and Williams (2005), and see Higdon et al. (2008) for a complete description of the emulators constructed here.”

L85: I do not understand what is meant by: “in terms of the proportion of output variance corresponding: to each GlaDS parameter”. Please clarify.
What we mean to say here is that we used the emulators to determine how each parameter influences the GlaDS outputs. We have clarified this statement to: “Following tuning and evaluation of the emulator, we apply the emulator to quantify the relationship between GlaDS parameters and GlaDS output.” We provide a full technical definition, now including defining equations, in Section 5.

L91: Rephrase: Let $\mathbf{y}_i$ denote the vectorized model output of all variables (...).
If we understand the reviewer correctly, it appears that this statement was suggesting that we were concatenating the variables into a joint vector. Here, we intend $\mathbf{y}_i$ to be a placeholder for a single variable (e.g., flotation fraction). We have clarified this in the text by letting “$\mathbf{y}_i$ denote the vectorized model output of interest”.

L94: Typo: “which are not a part of”.
It appears the reviewer is pointing out the typo that it is incorrect to refer to $\mathbf{y}_i$ as the prediction for new parameter values since $\mathbf{y}_i$ is previously defined as the output corresponding to parameters $\mathbf{x}_i$. We will avoid overloading $\mathbf{y}_i$ by writing that “The emulation task is to predict the simulation output for new input values which are not a part of the design matrix $\mathbf{X}$”. Elsewhere, we use $\mathbf{y}_p$ to represent the emulator prediction.

L104 Add a comma after $\boldsymbol{\theta}$.
If we are interpreting this suggestion correctly, it was unclear whether the hyperparameters were associated with the covariance function or with the mean function. We have reversed the ordering of the mean function and covariance function in this sentence to avoid this potential source of ambiguity:

"The GP is completely specified by the mean function μ(x) and the covariance function $k(x_i, x_j; \theta)$ with hyperparameters θ".

L110: Refer to $\mu(x)$ after "mean function".
Thank you for catching this, we will ensure to refer to variable symbols after their names throughout the text.

L110: "to set the mean to zero" should be to set the prior mean to zero. In the following sentences, it is also important to emphasize that it is only the prior mean that is zero.
Thank you for suggesting this technical correction, we have changed the quoted statement to: "to set the prior mean to zero", with corresponding changes throughout this section.

Eq. (5): This should be $y_p | \mathbf{Y}, \boldsymbol{\theta}, x_p$
Thank you for catching this mistake, we have corrected this as indicated

L124: I recommend being more specific here: (...) contains the pair-wise covariances between x_p and each: entry of x (...).
This is a good suggestion to clarify that $\boldsymbol{k}_p$ is also a pairwise covariance vector. However, we would like to emphasize that the covariance function k represents covariance between model outputs, not covariance between model parameters. We have now clarified that "the vector $k_p = k(x_p, x)$ contains the pairwise covariance between the model outputs from the simulation ensemble and the estimated output for parameters x_p".

L126: Specify: The prediction mean
Done.

L127: Refer to Eq. (4) after "covariance function".
Good suggestion, done.

L136 and L137: Replace "will" by would.
Done.

L138: Typo: "a variety solutions".
Corrected: "a variety of solutions".

L148: Please specify here that Eq. (8) assumes uncorrelated errors. This may not be entirely valid in this case.
The reviewer is correct, this has been revised to acknowledge that "This error model assumes that errors at each spatial position and timestep are uncorrelated, which might not be strictly true for our application."

L152: "can be viewed as": this wording is inappropriate, because it is a dimension reduction by definition.
We have added a more direct statement about the PC decomposition to the beginning of this paragraph: "In order to reduce the dimensionality of the simulation outputs, which leads to the obstacles described

above, the multivariate output field is modelled directly by using a principal component (PC) decomposition.”. We were trying to be cautious not to lead the readers to think that a PC decomposition is the only way to address the size of model outputs.

L162: The authors can also invoke the orthogonality property of the PC decomposition to motivate their univariate approach.
Good suggestion, we have added the explanation: “Following Higdon et al. (2008), since the PCs are orthogonal, independent univariate GPs are fit to model the relationship between the inputs…”

L169: Replace “permissive” by flexible.
We prefer “permissive” since, in our view, one reason to use a covariance function with a weaker smoothness constraint is to permit a larger class of random functions. “Permissive” reflects this effect on the space of random functions.

L169: “variations in the principal components that tend to be smooth with respect to the input parameters”: why is that? I would expect a strong sensitivity of GlaDS to some of its parameters, even in the PC subspace. Could the authors please clarify this statement?
We would like to clarify that strong sensitivity does not imply non-smoothness. The PC value can have large variations as parameters are varied. As long as these variations are reasonably smooth, the squared-exponential kernel is a reasonable choice. For clarity, we have revised this statement to: “While the flotation fraction field need not be smooth in space and in time, the principal components w_{ij} (θ) tend to vary smoothly with respect to the GlaDS parameters since the the spatiotemporal complexity is captured by the principal component basis.”

L173: How many GP realizations are sampled?
We draw 64 GP realizations to compute the mean and prediction quantiles for these comparisons. We have found the mean and quantiles to be reasonably converged with this number of samples. For the more detailed evaluation of the reference emulator, we use 512 GP realizations. We have added this detail to this line.

L179-181: I am not sure to agree here. As I understand it, each univariate GP is fitted to a single series of PC coefficient, regardless of the number p of PCs retained. The number of parameters scales linearly with p, being p(d + 1) + 1. However, the amount of data used for fitting also scales linearly with p, because increasing p by 1 implies that one more series of PC coefficients is used. As such, I do not see why “a simpler model with fewer PCs and therefore fewer hyperparameters to estimate is desirable as it will have less prediction variance (i.e., less tendency to overfit)”. On the other hand, I believe that using an increasingly high number of PCs would imply increasingly many GPs fitted to low-variance component of the GlaDS output, which can be regarded as noisy features of GlaDS results rather than dominant components of the variability.
The reviewer is right in saying that we are expanding the amount of data used in training each time we increase the number of principal components (p). Since the individual GPs are independent, each receives a different orthogonal vector of PCs that are used to infer the hyperparameters for that particular GP. Adding another GP therefore means that we use an additional column of the PC matrix to fit another set of hyperparameters. As in Higdon et al. (2008), we find that GP prediction ability levels off beyond a

certain number of principal components *p* (Fig. 3, 4). We have updated this statement accordingly: “In practice, GP predictions can be less accurate for later principal components that explain a small fraction of the ensemble variance (e.g., Higdon et al., 2008). Since including GPs for these later PCs does not meaningfully improve predictions, we will select a model with a modest number of principal components that nonetheless has similar performance obtained by using more components.

Section 3.1: In general, I think that more details are needed in this Section.
We have added details throughout this section as detailed in the following responses.

L192: Add one sentence to explain what the K-transect is.
We have described the K-transect as part of the western Greenland Ice Sheet.

L192-193: “adjusted from 0 m” and “increased to 40–1560 m”: are these adjectives with respect to the SHMIP configuration? If so, please specify.
We have clarified these adjustments to: “The synthetic geometry consists of a flat bed with an elevation of 350 m (adjusted from 0 m in the SHMIP experiment) and surface elevation between 390–1909 m (adjusted from 1–1520 m in the SHMIP experiment) to match the observed elevation range of this part of the ice sheet.”

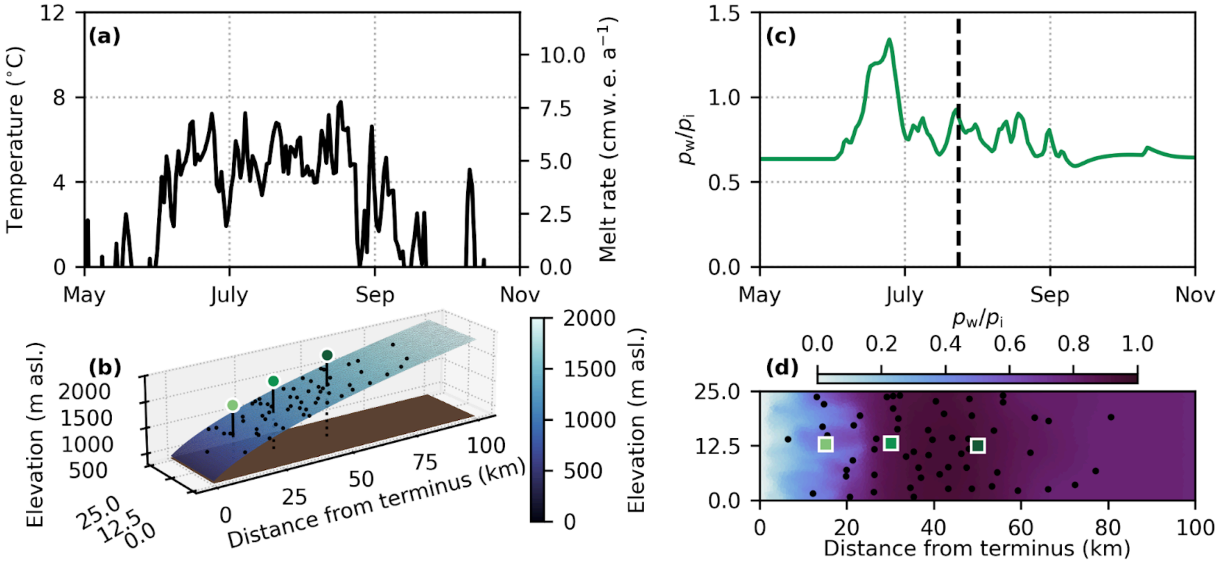
L196: Please put the basal melt rate imposed into a glaciological context. For example, how does it compare with basal melt rate estimates in Greenland, or with the SHMIP forcing?
We have added that “This basal melt rate is in line with modelled basal melt rates in western Greenland (e.g., 0.001–0.1 m w.e. a−1, Karlsson et al., 2021), but lacks the seasonality associated with basal sliding”. We have omitted a comparison to the SHMIP basal melt forcing since comparing the prescribed melt rates to the Karlsson et al. (2021) model results is a more robust comparison.

L199: “ following a moulin density that varies with elevation computed from a satellite-derived supraglacial drainage map”: is it possible to provide the formulation of the moulin density as a function of elevation?
We have added that “moulin density is parameterized by a normal distribution with mean 1138 m and standard deviation 280 m”.

L200: “within each sub-catchment”: this is not explained.
We have added an explanation that surface catchments are defined by a Voronoi diagram: “Surface melt is accumulated within sub-catchments surrounding each moulin defined by a Voronoi diagram and instantaneously routed to the bed.”

Figure 1 Is it possible to add the melt rate using the right y-axis in Fig. 1a? What does the color scheme represent in Fig. 1b? Is it possible to indicate the moulin locations in Fig. 1d?
We have updated Figure 1 to include:

- A right y-axis on (a) to indicate surface melt rate
- A colorbar for (b) (surface elevation, m asl.)
- Moulin positions on (b) and (d)



L203: Replace “posed” by configured.

We have kept “posed” as this is the language used by Werder et al. (2013) to originally describe the discretization of the model on a triangular unstructured mesh.

L204: The variable x is already used to denote the input to the GPs. Please do not use the same symbol for two different variables.

Good point, this reference to x is unnecessary since we do not refer to x elsewhere, so we have removed “x=0 km” from the description of boundary conditions.

L216: “Following the vocabulary of Higdon et al. (2008) and Verjans and Robel (2024)”: this is not needed here.

Following our response to General comment (2), it has sometimes been helpful to use “emulator inputs” rather than “GlaDS parameters” when talking about GP emulators more abstractly. We have moved this statement ahead to the beginning of Section 2 to explain these different terms before they are used.

L222: Concerning the parameter ranges, the ranges provided in Table 2 are most likely not intuitive to a majority of readers. I recommend adding a column in Table 2 specifying the ranges of parameter values used in previous studies focused on uncertainty quantification from GlaDS parametric uncertainty (e.g., Brinkerhoff et al., 2021).

We fear such an addition would be misleading, rather than helpful, as only two of the parameters (channel conductivity k_c and bed bump aspect ratio r_b) correspond one-to-one with Brinkerhoff et al. (2021), who varied fewer subglacial drainage model parameters and used different cavity-opening and sheet-flow parameterizations. We have therefore not made this change.

L223: “flotation fraction fw < −10”: in principle, any fw < 0 is nonphysical because it implies pw < 0. Are all these simulations rejected from the training data? And/or is the GP constrained to predict pw > 0?

It is correct that any flotation fraction f_w<0 is nonphysical since the model does not include physics for open-channel flow. We do not reject simulations from the training data, we sample from the entire hyper-rectangle described by Table 2. We do not constrain the GP predictions since the goal of this work is to produce an emulator that mimics the model of choice (GlaDS) as closely as possible. We have clarified this description in the text: “We sample from the entire region described by the bounds listed in Table 2 without filtering or discarding nonphysical training runs (c.f., Jantre et al., 2024). The ensemble still contains some instances of negative or extremely high flotation fraction, but these do not appear to negatively impact the principal component decomposition nor the emulator predictions.”

L234: As I understand, the test data do not include any extrapolation beyond the parameter space used for training. Therefore, it should be mentioned here and in the Discussion that the extrapolation capability of the GP emulator has not been evaluated.
This is correct, we have not evaluated the parametric extrapolation capability. When modelling a deterministic process (e.g., computer model outputs) with scalar GPs, there is a clear notion of interpolation. While it is not as clear in our case using the truncated basis representation, we still view the GP as interpolating between the training simulations to make predictions for new inputs. With this interpretation, we explicitly want to avoid extrapolating outside the range of parameters used in the GlaDS ensemble. We have acknowledged this in Section 6.1 after discussing the performance of the GP on the test data:
“Emulator performance has not been assessed when extrapolating outside of the range of parameters used for training the model. For predictions far outside the training range, the zero-mean GP that we have used will revert to predicting the mean of the ensemble of simulations, likely producing significantly higher error than we have found on the test data. Predictions should therefore only be made within the parameter ranges used in the GlaDS simulation ensemble.”

L242: Please change this sentence to “In addition to emulating the spatiotemporal flotation fraction, (...)”.
Done.

L277: Remove “small”.
Removed since this section acts as the Results and we want to avoid much interpretation here.

L279: “perhaps since the input space has been explored more thoroughly”: I do not think this is the case. In my view, more PCs are needed simply because the rank of the output space increases. For example, if a single simulation is run, it is fully characterized by a single PC. As more simulations are included, the number of PCs required to fully characterize the outputs increases, and thus the number of PCs to characterize a given % of the output variance also increases.
I think that we may have the same ideas about the size of the output space and the number of PCs. By exploring the input space more (i.e., running more simulations, including further towards the edges and the corners of parameter space), we obtain more linearly independent simulations, increasing the rank of the output space. We have found that the number of PCs needed to obtain a certain RMSE or cumulative variance threshold does not exactly scale with the number of simulations in the ensemble. For example, by doubling the number of simulations from 256 to 512, we do not need to double the number of PCs to maintain a consistent variance threshold. We have therefore not made any changes to this description.

L284: “only the absolute value, not the sign, of the PC basis vectors should be interpreted”: I disagree. Opposite signs indicate opposite phasing of variability. It would be more correct to say that the sign of any given PC basis vector is arbitrary, but only looking at the absolute value would be wrong.
That is correct, we have updated this statement as suggested: “Note that the sign of the PCs and basis vectors are arbitrary since inverting the sign of both the basis […]”

Figure 3: Specify if the lines show the mean or median of RMSE and MAPE taken across the test simulations.
Lines show the median RMSE and MAPE across the test set. This caption has been revised to “Median root mean square error (RMSE, a) and mean absolute percent error (MAPE, b) for GP emulator predictions across the 100 test inputs [...]”

Figure 4c,f: I think that the presentation of the 95% prediction intervals is both unclear and misleading. Firstly, I understand that the RMSE and MAPE boxplots show the errors averaged in both time and space. But for the 95% prediction intervals, do the boxplots show the entire population of 95% prediction intervals taken at each grid cell and each time step of each test simulation?
We have clarified that a–c “show the distribution of the RMSE, MAPE and the spatiotemporally averaged 95% prediction interval evaluated on the test ensemble”

Secondly, this Figure suggests that broad prediction intervals are a bad thing. However, the purpose of a prediction interval is to communicate about the uncertainty in the output. Thus, it is a good thing that prediction intervals are broader for cases with high RMSE (i.e., the simulations with low PC numbers in this Figure). This means that the true GlaDS value may still lie within the 95% prediction interval despite the larger error in the mean estimate. For this reason, I recommend to show the percentage of GlaDS values falling outside of the 95% prediction intervals in Figure 4c,f, rather than the 95% prediction intervals themselves. If the GPs are well-calibrated, this percentage should be 5%.
We agree that broad prediction intervals are good if the breadth is necessary to encompass the expected proportion of the simulated values. We have added Fig. B4 (copied below) that presents the proportion of emulator-predicted values that overlap the simulated values.

We agree with the reviewer that the most important point is accurately communicating uncertainty in the emulator predictions. In presenting Fig. 4 and interpreting its results, we have not interpreted higher prediction uncertainty to be necessarily good or bad. Considering that Fig. B4 (copied below) shows the emulator uncertainty intervals contain the expected proportion of simulated values (i.e., are well-calibrated), we use the width of the prediction intervals to illustrate how adding more training simulations narrows the spread of predictions. If the intervals are properly calibrated (as shown by Fig. C3), then the balance between prediction uncertainty and cost to run the ensembles can be an important choice.

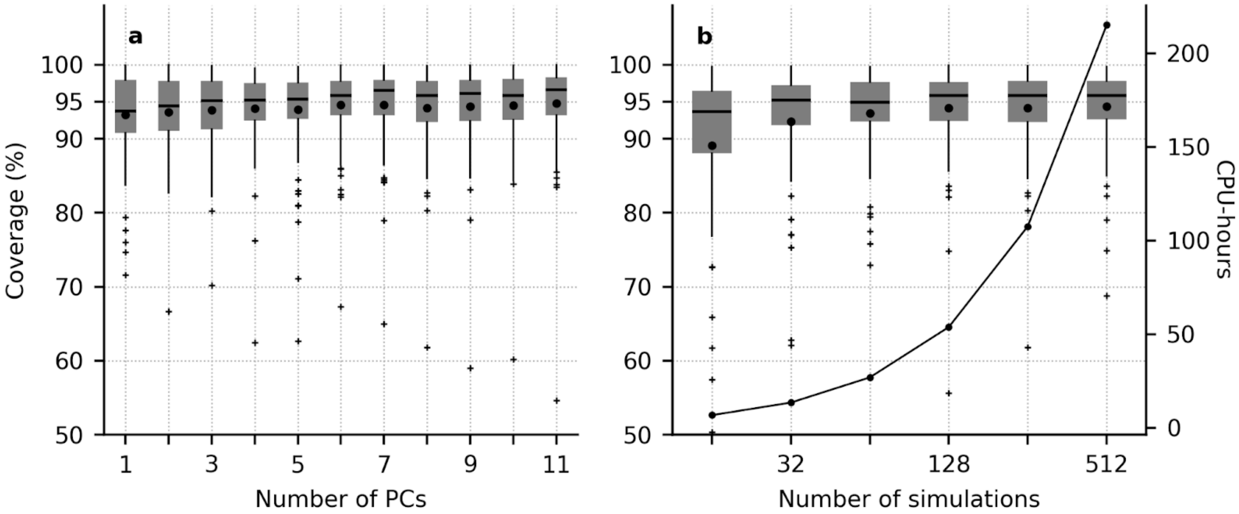


Figure: Proportion of GP emulator-predicted flotation fraction values that overlap the simulated values within the 95% prediction interval across the test set. (a) For emulators constructed using different numbers of principal components. (b) For emulators using subsets of the training ensemble. Horizontal lines indicate the median and black dots indicate the mean across the test set. The right axis in (b) indicates the number of CPU-hours associated with running each subset of the GlaDS training ensemble.

Figure 4d,e,f: Please mention in the caption that the x-axis uses a logarithmic scale.
Added.

Figure 4 caption: “Black circles indicate the total integrated prediction uncertainty”: I do not understand this.
Since GP uncertainty varies with the distance to training points, we wondered if using the median uncertainty at the test points would overestimate the true mean if the test points were unusually far from training points. We assessed this by a Monte Carlo integral of the 95% prediction spread across the space of 8 GlaDS parameters. It is encouraging that the black circles (Monte Carlo-integrated) are near the median, as this shows that the test points are representative in terms of their prediction uncertainty. We have added the following explanation to the text: “Since GP prediction uncertainty varies across the space of emulator inputs depending on the distance to training runs, we assess the overall prediction uncertainty by computing a Monte Carlo integral across the space of GlaDS parameters, indicated as black circles in Fig. 4c”

L320: I find that it is worth mentioning that the RMSE for the three GPs is very similar for the late-September melt event, and I suggest to provide a succinct explanation of why this is.
This is a good observation. We have added an acknowledgement of this in the text: “All models have a similar RMSE during the September melt event, with relatively little improvement obtained by including more PCs.” We do not have a concise explanation of why this event appears to be hard for the emulator to capture. Late-season melt events have persistently been difficult for the emulator, including in more recent work that uses different melt forcing and realistic geometry (preprint: https://doi.org/10.31223/X5GQ68). Observations of ice-sheet surface velocity show a similar type of strong response to moderate surface melt rates at the end of the melt season (e.g., Andrews et al. (2014)

Extended Data Figure 1c) as the drainage system is shutting down, suggesting this is an especially sensitive time for the drainage system.

L321: Typo: “reduces by the height”.
Corrected: “Using 8 PCs reduces the height of”

L335: Table C1 should be referenced here.
We have added this reference.

L337: Please explain why fw > 2 is considered unrealistic.
We mean to say that any f_w>1 other than short-duration, highly localized events is unrealistic. We were using f_w>2 as an example. To clarify, we have revised this to say “many of the GlaDS simulations produce unrealistically high water pressure exceeding overburden (fw $\gg$ 1) for long periods of time and over a large portion of the domain (e.g., Fig. 6a2 and Fig. 7a2, b2)”.

L343: “suggesting the emulator has reasonably accounted for basis truncation error”: please note that this also suggests that the GP can correctly estimate uncertainty due to interpolation towards unseen parameter values.
Correct, this has been changed to “interpolation and basis truncation error”

L345: Add comma after “spring”.
Thank you for the suggestion, we have added the indicated comma and revised this sentence to: “In the higher-error simulation, however, the prediction intervals do not overlap the simulation outputs in ~~the~~ spring**,** when the mean prediction significantly overestimates flotation fraction”.

L345: “the mean prediction significantly overestimates flotation fraction”: this suggests that the GP tends to further amplify the unrealistic GlaDS output. Please mention this explicitly.
We have added: “In other words, the emulator has amplified the unrealistically high GlaDS flotation fraction in the case of the 95th-percentile RMSE test simulation.”

Table 3: Specify: Single GlaDS simulation.
Added.

L353 and Figure 8: Please use coefficient of determination (R^2) as an evaluation metric, rather than the squared correlation coefficient (r^2).
We have updated the analysis to compute the coefficient of determination (R^2) instead of the squared correlation coefficient (r^2).

L350-359 and Figure 8: These comparisons are misleading, because the GP emulator has been trained to reproduce f_w. It is impossible to know what the performance of the GP would be if it had been trained to reproduce ϕ or N. The discussion here should be rephrased as an evaluation of the error introduced by the conversion from fw to ϕ and/or N, rather than “indicators of GP prediction performance” or “different prediction skill” (L355).

Our main claim is that converting from one measure of water pressure to another will change the performance metrics of emulator predictions, as shown by Fig. 8. Based on this evidence, we suggest to emulate and train using the variable of interest for the study at hand. By converting emulator and simulator outputs to different units, we find that the hydraulic potential is the weakest of the three indicators of prediction skill since this comparison yields the highest proportion of explained variance (99.3%) when identical simulations and predictions are being compared. We have revised the text to ensure the accuracy of our statements. We would like to emphasize that we do not make any claims about the behaviour of hypothetical emulators constructed to predict effective pressure or hydraulic potential directly.

Figure 9 column c: Same comment concerning the prediction intervals as for Figure 4c,f.
As with our discussion of Fig. 4, the results and discussion section corresponding to this figure use reductions in prediction uncertainty as an example of why one might want to run additional simulations even as RMSE and MAPE are nearly stationary as long as the uncertainty estimates are well-calibrated.

L368: “Based on RMSE, MAPE and bias”: I am not sure that these performances can be compared so easily from Table 4. For example, RMSE and bias have different units for the three variables. MAPE could serve as a better comparison basis, but Ts has been log-transformed, and MAPE may not be representative of the error on Ts itself. In addition, as mentioned by the authors, the MAPE values depend on the degree of variability in each quantity and on the values themselves (e.g., the percentage error when log Ts is 0 tends to infinity). Finally, when considering the ranges of values provided in Table 4, it is not clear to me that “the channel discharge fraction emulator has the best performance”.
This is a good point. As the later part of the reviewer’s comment indicates, this comparison should only be based on MAPE since the units of these quantities are different. We have refined this statement to more precisely relate to percent error, and not include broad statements about performance for such different quantities:
“We obtain the lowest percent error for the channel discharge fraction emulator (MAPE 5.02%), with similar percent error for the sheet transit time and channel network length emulators (8.7%; Table 4)”

L389: “Sensitivity indices for the flotation field are defined as a variance-weighted sum of the sensitivity indices for each principal component”: This one-sentence explanation is not clear to me. If possible, I recommend providing the mathematical formulation for the sensitivity indices. That is, which formula is used to compute the values shown in Figure 10? Furthermore, the difference between first-order and total sensitivity indices should be explained.
We have added equations defining the sensitivity indices and expanded the description of how we compute sensitivity indices for the flotation fraction field.

Figures 10 and 11: Some whiskers extend beyond the value of 1.0. While the value of 0 can be intuitively interpreted as no sensitivity, what do values >1.0 mean?
These are errors from using only a finite number of GP predictions in estimating the sensitivity indices. The Saltelli et al. (2010) estimators that we use are guaranteed to converge as the number of simulations tends to infinity. In practice, the bootstrap sampling finds subsets where predictions holding certain parameters fixed have a higher variance than predictions with all parameters varying. We have added a brief description of the error bars, which was missing in the earlier version

“Confidence intervals for the sensitivity estimates are computed by bootstrap resampling. Confidence intervals extending >1 are a result of numerical errors in the estimators, which are only guaranteed to converge in the limit of infinite simulation runs (Saltelli et al., 2010)”

L418: “prediction RMSE is < 20% of the ensemble standard deviation”: across the 100 test simulations? Yes, we have clarified this detail: “Across the input space, prediction errors are small relative to the variations across the ensemble of simulations: prediction RMSE is <20% of the standard deviation of the 100-member test ensemble”

L422: “PC truncation RMSE on the test set for the reference model with 8 PCs is 0.034, while GP prediction RMSE is 0.054, suggesting the PC truncation error contributes more than half of the prediction error.”: I think that this statement requires a more thorough justification, and I am also not sure that I agree with the authors about it. First, does the 0.034 value correspond to the case of 8 PCs for the curve 256 simulations in Figure 2a1? If so, please refer to Fig. 2a1 in the text. Second, Figure 4 shows that there seems to be a baseline RMSE of the GP predictions of about 0.05, which does not decrease when going from 7 to 11 PCs. On the other hand, the PC truncation error must decrease when going from 7 to 11 PCs. As such, this indicates that there is a balance between (1) using only the first few PCs that seem to be relatively easy to predict for the GP, and (2) including low-variance PCs that allow to reduce the truncation error, but that seem to be harder to predict for the GP. As a consequence of this balance, the baseline RMSE stagnates at 0.05. But saying that “Of the two error sources, PC truncation error is the larger contributor” is misleading. I believe that if more PCs had been included, PC truncation error would decrease, but GP error would increase. Thus, this conclusion seems to be due to the choice of truncating at 8 PCs, rather than an inherent attribute of the GP. At least, this is how I understand the results. I would welcome any thoughts from the authors about this.
The reviewer is correct, and we were not clear in the text that these statements are only about the p=8 reference emulator. We have identified that we are talking about the reference emulator and acknowledged that “the balance between basis truncation error and GP error depends on the number of principal components used”.

L434: “5 − 10 × 10^4 time steps”: why such a range? I thought that all simulations had been performed over the same time period and with the same temporal discretization.
This was unclear: we were adding up the time steps across the whole ensemble, i.e. up to 512 x 365 time steps. We have clarified: “This ensemble contain a large volume of data: the ensemble consists of up to 512 simulations, each with 365 time steps and ~4000 nodes”

L446: “The impact of large errors in predicting the spring pressure maximum is also reduced for ice-flow modelling applications”: I disagree with this statement. For example, Fig. 4d (magenta curve) and Fig. S4c of Verjans and Robel (2024) show that the highest ice flow velocity errors due to the subglacial hydrology emulation occurs in the spring pressure maximum (their Fig. 4d) and at the ice velocity peaks (their Fig. S4c), which generally coincide with the spring pressure maximum. So, it is impossible to verify this claim from the authors if they do not actually compare ice flow model realizations forced with the GlaDS versus the GP output.
Thank you for pointing out that our original statement, definitively saying that errors associated with the spring pressure maximum will be reduced for ice-flow applications, was too strong. We have changed this

to suggest that errors “may be reduced” and clarified that “The impact of large errors in predicting the spring pressure maximum may be reduced for ice-flow modelling applications if the difference is only in the amplitude and not the duration of the pressure maximum.”, with the explicit acknowledgement that “errors in the duration of water pressure exceeding the prescribed cap would propagate through the ice-sheet model to produce discrepancy to some extent in modelled velocity fields relative to using GlaDS directly”.

L454-455: “ the model of Verjans and Robel (2024), who report squared correlations (r^2)”: this is not correct. Verjans and Robel (2024) report the coefficient of determination (R^2), which is not the same metric as r^2.
Thank you for correcting us, we have updated this to the coefficient of determination (R^2).

L474: “since PC truncation typically preferentially dampens high-frequency variations”: I disagree with the authors here. PC truncation selects the components of variability with maximum variance. If most of the variance lies in high-frequency bands of the spectrum, there would not be any damping of high-frequency variations. Whether PC truncations dampens high-frequency variability or not depends on the power spectrum of the data.
The reviewer is correct. This statement was coming from our observations in previous work that using higher-frequency melt forcing results in larger differences between simulations with different parameter values relative to lower-frequency melt forcing (Hill et al., 2024). Based on this, we expect that using lower-frequency melt forcing would lead to a more accurate truncated basis representation in terms of RMSE. We have changed this statement to: “Smoother, averaged melt inputs (e.g., monthly, Table 5) would likely lead to reduced PC truncation error and therefore more accurate GP predictions since GlaDS simulations tend to have smaller variations in time and between simulations with lower-frequency melt inputs (Hill et al., 2024)”

L477-479 It is also important for resolving sub-annual ice flow variability.
That is correct, but since we do not include an ice flow component to this study, this paragraph focuses on implications for subglacial drainage models only.

L487: I believe that it would be relevant to add a sentence here about the propensity of GlaDS to produce nonphysical output.
This is another compelling reason that physics-based machine learning for GlaDS outputs has uncertain benefits. We have added this point to this section: “Considering the discontinuous nature of the channelized drainage system and the tendency of GlaDS to produce unrealistically high water pressure, it remains an open problem to apply physical constraints, such as mass conservation, to the subglacial drainage model emulation task and determine the applications which would benefit from such constraints.”

L493: Citing Verjans and Robel (2024) here is misleading, because their emulator is transferable to different domains or melt inputs, i.e., the opposite of the sentence given here.
That is correct, this citation should be (c.f., Verjans and Robel, 2024) to highlight that we are contrasting these approaches. As part of answering another reviewer’s comments, we have added a more nuanced

discussion to Section 6.4 of the applications that each of the three emulation studies (this study; Brinkerhoff et al., 2021; Verjans and Robel, 2024) are best-suited for.

L521-528: I found this entire paragraph a little vague and hand-waving. I recommend that the authors focus on the current work and future developments. For example, why discussing emulator predictions of global mean sea-level rise? This is clearly not the focus of this study.
This paragraph was intended to convey some of the decision points reached when designing an emulator, using applications taken from a wider swath of glaciology. We have removed the reference to sea-level rise contributions since that was distracting. As part of answering another reviewer's comments, we have added a paragraph discussing specific applications that are well-suited for the GP emulator approach that we have presented. Hopefully this paragraph will help address the vagueness highlighted by the reviewer.

L542: Typo: "is is".
Corrected.

L548-549: "fully Bayesian time-dependent calibration to provide observationally constrained distributions of subglacial drainage variables": I do not understand what the authors mean here.
We have clarified that we mean "Bayesian calibration with spatiotemporally resolved data to infer constrained distributions of subglacial drainage variables."

L561-562: Add regimes after "laminar and turbulent".
Done.

Eq. A3: To make the notation less clumsy, I suggest replacing the third and fourth terms on the left-hand side by $\partial h/\partial t$.
Since both forms are technically correct, we have intentionally duplicated the terms to provide the most explicit representation of the governing equations.

L603: Please specify: of a multivariate Normal distribution.
Added.

Eq. B3: For this equation to be valid, there needs to be an additional constant term on the right-hand-side.
Thank you for highlighting that we were slightly abusing notation here. As part of reviewer 3's comments, we have brought the appendix B content into the main text and we no longer include this log-likelihood equation. In the corresponding likelihood equation in the main text (now Eq. (11)), we have provided the complete likelihood including all constants to provide a direct visual analogy to the univariate GP likelihood, Eq. (9).

L616: Typo: "includes" should be include.
Corrected.

L625: Typo: "by condition" should be by conditioning.
Corrected.

Eq. B5: θ should be boldfaced.
Corrected.

L629: then sampling from equation (B5)
Thank you for checking our equation references. Equation (5), the GP posterior predictive distribution, is the correct reference here.

L634: a major benefit of using
Corrected.

L635: Can the authors please remind here what are p and d so that the reader does not need to go back to the main text?
This is a good suggestion, and we should also not be using *p* (the number of PCs) here since this is the extension of the univariate GP section. We have changed this to *d*+1 "where d=8 is the number of GlaDS parameters".

Figure C2: It seems to me that some of the Markov Chains are not well-mixed, although it is hard to tell from the scale of the y-axes. Did the authors compute convergence diagnostics? I recommend providing R-hat values and effective sample sizes (Gelman et al., 2013).
Thank you for the good suggestion. We have now computed the R-hat values and effective sample size N_{eff} according to Gelman et al. (2013, p. 284–287). The median R-hat (1.065) and median effective sample size N_{eff} (58 using 4 chains) indicate reasonable convergence. However, chains for individual parameters have not converged with R-hat as high as 1.3 (corresponding to h_b for PC2) and N_{eff} as low as 13 (corresponding to k_c for PC8). Based on these diagnostics, we will:

1. re-investigate the step sizes used in the MCMC to ensure that the acceptance rates are in an appropriate range (~20–50%),
2. extend the length of the MCMC chains to ensure that chains are reasonably converged (as measured by R-hat) and that they contain a sufficient number of independent samples (as measured by N_{eff}),
3. report the acceptance rate, R-hat and effective sample sizes in the revised manuscript.

Figure C3: These figures should be shown in two dimensions rather than 3 for better clarity.
Part of the intention of this figure was to visualize the parameter interactions, which is best presented in 3D perspective. We understand the ambiguity in 3D plots with a single perspective, but we hope the surfaces are clear enough since we have added the colour scale to indicate the value (i.e., height) of the scalar quantities.

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