Extending GLUE with Multilevel Methods to Accelerate Statistical Inversion of Hydrological Models

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Key Points:

- Generalized Likelihood Uncertainty Estimation (GLUE) is extended to a setting with multiple levels of model accuracy (MLGLUE)
- MLGLUE reduced the time of inversion for a groundwater flow model by $\approx 45\%$ and $\approx 57\%$ compared to GLUE and standard Markov-chain Monte Carlo
- MLGLUE is especially well-suited for models that discretize independent variables but is shown to be applicable in more general settings

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Abstract

Inverse problems are ubiquitous in hydrological modelling for parameter estimation, system understanding, sustainable water resources management, and the operation of digital twins. While statistical inversion is especially popular, its sampling-based nature often inhibits the inversion of computationally costly models, which has compromised the use of the Generalized Likelihood Uncertainty Estimation (GLUE) methodology, e.g., for spatially distributed (partial) differential equation based models. In this study we introduce multilevel GLUE (MLGLUE), which alleviates the computational burden of statistical inversion by utilizing a hierarchy of model resolutions. Inspired by multilevel Monte Carlo, most parameter samples are evaluated on lower levels with computationally cheap low-resolution models and only samples associated with a likelihood above a certain threshold are subsequently passed to higher levels with costly high-resolution models for evaluation. Inferences are made at the level of the highest-resolution model but substantial computational savings are achieved by discarding samples with low likelihood already on levels with low resolution and low computational cost. Two test problems demonstrate the similarity of inferred parameter posteriors and uncertainty estimates of MLGLUE and GLUE as well as increased computational efficiency. Findings are furthermore compared to inversion results from Markov-chain Monte Carlo (MCMC) and from multilevel delayed acceptance MCMC. The computation time of inversion of a groundwater flow model was decreases by $\approx 45\%$ and $\approx 57\%$ when using MLGLUE instead of conventional formulations of GLUE and MCMC, respectively.

1 Introduction

Inverse problems are ubiquitous in hydrological modelling, emerging in the context of parameter estimation, system understanding, sustainable water resources management, and the operation of digital twins (e.g., Leopoldina, 2022). Inverse problems in this context are often severely ill-posed, resulting in uncertainties associated with computational models (Beven, 1993; Carrera et al., 2005; Beven, 2006; Vrugt et al., 2009; Zhou et al., 2014; Mai, 2023). Considering hydrological system complexity and limited data availability, these uncertainties therefore need to be quantified (Blöschl et al., 2019). While process-based spatially distributed models are often needed to adequately guide decision-making and to sustainably manage water resources, such modelling approaches are computationally costly (Doherty, 2015; Herrera et al., 2022), making uncertainty quantification (UQ) and statistical inversion especially challenging (Erdal & Cirpka, 2020; Kuffour et al., 2020; White, Hunt, et al., 2020). There is a need to develop computationally efficient approaches to UQ and statistical inversion to overcome the pressing challenges associated with climate change and their impact on water resources.

Various approaches to UQ have been developed and applied in that respect; the Bayesian approach to statistical inversion and UQ, however, is especially popular due to the ability to comprehensively treat uncertainties in state variables, parameters, and model output (Montanari, 2007; Vrugt, 2016; Linde et al., 2017; Page et al., 2023). Gen-

eralized Likelihood Uncertainty Estimation (GLUE) (Beven & Binley, 1992, 2014; Mirzaei et al., 2015) - as an informal Bayesian approach - and Markov-chain Monte Carlo sampling (MCMC) (Gallagher et al., 2009; Vrugt, 2016; Dodwell et al., 2019; Brunetti et al., 2023; Lykkegaard et al., 2023) - as a formal Bayesian approach - are frequently applied in the environmental sciences for statistical inversion. The Bayesian framework considers model parameters to be random variables that are associated with a prior distribution, which is conditioned on system state observations using a likelihood function to form a posterior distribution. The likelihood function may either be defined formally (often requiring knowledge about sources of model error as well as assuming independent and identically distributed errors) or informally (aggregating all apects of error to a generalized fuzzy belief) (Beven & Binley, 1992; Beven & Freer, 2001). Alternatively, likelihood-free methods such as approximate Bayesian computation may be used (Nott et al., 2012; Sadegh & Vrugt, 2013; Beven, 2016; Vrugt & Beven, 2018).

Approaches to statistical inversion generally rely on repeatedly running the computational model with different parameter values to obtain simulated equivalents of observations. With computationally costly models, this approach quickly becomes intractable and there is a need to develop more efficient sampling approaches for statistical inversion. Different approaches have been developed to reduce computational cost of inversion, such as using data-driven surrogate or reduced-order models (Doherty & Christensen, 2011; Asher et al., 2015; Burrows & Doherty, 2015; Linde et al., 2017; Gosses & Wöhling, 2019, 2021; Allgeier, 2022) during inversion, often run instead of the computationally costly high-fidelity model. Reducing model spatial resolution can reduce model complexity and computational cost in general and the effect of horizontal (Wildemeersch et al., 2014) as well as vertical (White, Knowling, & Moore, 2020) discretization in groundwater model performance has been studied before, also in the context of accelerating inversion (von Gunten et al., 2014).

Multilevel methods and multilevel Monte Carlo (MLMC) (Heinrich, 2001; Giles, 2008; Cliffe et al., 2011; Giles, 2015), with extensions to multilevel MCMC and multilevel delayed acceptance MCMC (MLMCMC and MLDA, respectively) (Dodwell et al., 2019; Lykkegaard et al., 2023), were previously introduced with a similar motivation. In the context of spatially distributed models, multilevel methods utilize multiple levels of spatial domain resolution. Together with the most finely discretized highest level model, also a number of more coarsely discretized lower level models are considered. Most solutions to the forward problem are then carried out on lower levels while the highest level model is called far less frequently, harbouring the potential for large savings in overall computation time. Contrary to surrogate- or reduced-order-model-aided approaches to UQ, multilevel methods make no additional simplifying assumptions about the model and the relevant processes are simulated directly on all levels of resolution. Another such contrast is that the coarsely discretized models are not used instead of the high-fidelity model but they are synergetically used together. Linde et al. (2017) summarize first applications of MLMC for the forward propagation of uncertainties in hydrogeology and

hydrogeophysics. We note that multilevel methods may be used regarding the discretization of any independent variable, such as spatial coordinates or time.

Previous applications of multilevel methods focussed on models with different spatial resolutions (Cliffe et al., 2011; Linde et al., 2017; Dodwell et al., 2019; Lykkegaard et al., 2023), entailing challenges with model parameterization at different resolutions. Geostatistical approaches are often used to (initially) parameterize spatially distributed groundwater flow- or other hydrological models, which simultaneously reduces overparameterization. To this end, utilizing point measurements of parameters or the combination with other predictor variables, Gaussian process regression is frequently used to generate conditioned parameter fields on arbitrary spatial resolution (Kitanidis & Vomvoris, 1983; Zimmerman et al., 1998; Zhou et al., 2014; Doherty, 2003). Unconditioned random fields are also often used, where parameter fields are generated on arbitrary spatial resolution (Y. Liu et al., 2019); using uncorrelated and spatially independent random variables, the Karhunen-Loéve expansion is often used to parameterize the random field (Cliffe et al., 2011; Dodwell et al., 2019; Lykkegaard et al., 2023). The definition of hydrological respose units or internally homogeneous zones of parameters represents another strategy for parameterization (Kumar et al., 2013; Zhou et al., 2014; Anderson et al., 2015; White, 2018). To better constrain the parameter space during inversion and to reduce the aggravating effect of overparameterization, regularization can be employed in combination with different parameterization strategies (Tonkin & Doherty, 2005; Moore & Doherty, 2006; Pokhrel et al., 2008; Moore et al., 2010). Parameter scaling can be used to transfer parameter fields from one spatial resolution to another. While there is no generally valid theory for upscaling (i.e., from fine to coarse grid) (Binley et al., 1989; Samaniego et al., 2010), various upscaling operators are used in practice (Binley et al., 1989; Samaniego et al., 2010; Colecchio et al., 2020).

While multilevel methods have previously been used to accelerate MCMC algorithms (Dodwell et al., 2019; Lykkegaard & Dodwell, 2022; Lykkegaard et al., 2023) in a formal Bayesian framework, it has not yet been attempted for GLUE. In this study, we utilize ideas from multilevel Monte Carlo strategies to accelerate statistical inversion of hydrological models with the GLUE methodology. After introducing multilevel GLUE (MLGLUE), two example inverse problems are considered. We subsequently apply conventional GLUE and MLGLUE as well as MCMC and MLDA to those problems and compare the results.

2 The Inverse Problem

Consider observations $\widetilde{\mathbf{Y}} = [\tilde{y}_1, \dots, \tilde{y}_k]^T \in \mathcal{Y} \subseteq \mathbb{R}^k$ of a real system, made with measurement error $\boldsymbol{\varepsilon} \in \mathbb{R}^k$. Also consider a model $\mathcal{F}$ that simulates the system response $\mathbf{Y} = [y_1, \dots, y_k]^T \in \mathcal{Y}$ corresponding to $\widetilde{\mathbf{Y}}$. The model output also depends on initial and boundary conditions $\mathcal{C}_i$ and $\mathcal{C}_b$, respectively, as well as on model parameters $\boldsymbol{\theta} \in \mathcal{X} \subseteq \mathbb{R}^n$

$$\widetilde{\mathbf{Y}} = \mathcal{F}(\boldsymbol{\theta}, \mathcal{C}_i, \mathcal{C}_b) + \boldsymbol{\varepsilon} := \mathcal{F}(\boldsymbol{\theta}) + \boldsymbol{\varepsilon} \tag{1}$$

$\mathcal{F} : \mathcal{C}_i, \mathcal{C}_b \rightarrow \mathbf{Y} \in \mathcal{Y}$ is closed by the parameter vector $\boldsymbol{\theta}$ (Kavetski et al., 2006; Vrugt et al., 2009), which is considered a random vector with an associated prior distribution $p_p(\boldsymbol{\theta})$. Solving the inverse problem in a Bayesian statistical framework means to obtain the posterior distribution of the parameters $p(\boldsymbol{\theta}|\widetilde{\mathbf{Y}})$ via Bayes' theorem

$$p(\boldsymbol{\theta}|\widetilde{\mathbf{Y}}) = \frac{p_p(\boldsymbol{\theta})p(\widetilde{\mathbf{Y}}|\boldsymbol{\theta})}{p(\widetilde{\mathbf{Y}})} \propto p_p(\boldsymbol{\theta})p(\widetilde{\mathbf{Y}}|\boldsymbol{\theta}) \tag{2}$$

where $p_p(\boldsymbol{\theta})$ is the prior parameter distribution, $p(\widetilde{\mathbf{Y}}|\boldsymbol{\theta})$ is the likelihood function, and $p(\widetilde{\mathbf{Y}})$ is the evidence.

Assuming that model errors $r_i = y_i - \tilde{y}_i$ are mutually independent and identically distributed (i.i.d.) and follow a Gaussian distribution with constant variance σ_r^2, the log-likelihood takes the form

$$\mathcal{L}(\boldsymbol{\theta}|\widetilde{\mathbf{Y}}) = -\frac{k}{2}\ln(2\pi) - \frac{k}{2}\ln(\sigma_r^2) - \frac{1}{2}\sigma_r^2 \cdot \sum_{i=1}^{k}(y_i - \tilde{y}_i)^2 \tag{3}$$

The assumptions of i.i.d. model errors, however, usually does not hold as hydrological model errors often exhibit strong autocorrelation and heteroscedasticity (see, e.g., Beven (2006) for a discussion). Beven and Freer (2001) and Vrugt et al. (2009) give alternative likelihood formulations that deal with those issues, often at the cost of additional hyperparameters.

2.1 Multilevel Methods

We will discuss the notion of multilevel methods from the perspective of multilevel Monte Carlo (MLMC), which is a method to efficiently compute the expectation of a quantity of interest that depends on (model) parameters (Heinrich, 2001; Giles, 2008; Cliffe et al., 2011; Giles, 2015). While MLMC is used for the forward propagation of uncertainty instead of inversion, it builds on a simple intuition that illustrates the idea behind MLGLUE.

As an example, consider the situation where we are given a parameter (posterior) distribution $p(\boldsymbol{\theta})$ and want to compute the expected value of the model output $\mathbf{Y} = \mathcal{F}(\boldsymbol{\theta})$ with respect to $p(\boldsymbol{\theta})$, which is a problem of propagating parameter uncertainty through the model. For simplicity and without loss of generality consider $\mathbf{Y} \in \mathbb{R}$ for the remainder of this section. Instead of one single model for the system, assume that there is a hierarchy of models (approximations) $\{\mathcal{F}_\ell\}_{\ell=0}^{\infty}$ such that $\widetilde{\mathbf{Y}} = \lim_{\ell\to\infty}\mathcal{F}_\ell$, where ℓ is the level index. We assume that the computational cost for evaluating $\mathcal{F}_\ell$ increases while the approximation error decreases as $\ell \rightarrow L$. In the context of PDE-based models, ℓ may be related to the grid size or time step length of the model, i.e., a larger ℓ corresponds to a structurally more accurate model. To estimate the expectation of $\mathbf{Y}$ efficiently, MLMC avoids the direct estimation of $\mathbb{E}[\mathcal{F}_L]$ on the highest level $\ell = L$. Instead, the correction of the estimation with respect to the next lower level is computed, based on the linearity of expectation:

$$\mathbb{E}[\mathcal{F}_L] = \mathbb{E}[\mathcal{F}_0] + \sum_{\ell=1}^{L}\mathbb{E}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}] \tag{4}$$

This approach generally results in substantial computational savings and different multilevel estimators for $\mathbb{E}[\mathcal{F}_L]$ exist (Giles, 2008; Cliffe et al., 2011; Giles, 2015; Dodwell et al., 2019; Lykkegaard et al., 2023). The original MLMC algorithm of Giles (2008) (as well as subsequently applied algorithms) takes a bottom-up approach, i.e., sampling is started on $\ell = 0$ and ℓ is only incremented if the algorithm has not yet converged on level ℓ. There, efficiency and variance reduction regarding the expectation of $\mathbf{Y}$ may be optimized by choosing an optimal refinement (e.g., the decrease of cell or time step size when going from ℓ to $\ell + 1$).

In the context of MLMC, the behaviour of the variances $\mathbb{V}[\mathcal{F}_\ell]$ and $\mathbb{V}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ and expectations $\mathbb{E}[\mathcal{F}_\ell]$ and $\mathbb{E}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ as $\ell \to L$ gives an indication of the overall quality and efficiency of the hierarchy $\{\mathcal{F}_\ell\}_{\ell=0}^{L}$ (Cliffe et al., 2011). $\mathbb{V}[\mathcal{F}_\ell]$ and $\mathbb{E}[\mathcal{F}_\ell]$ should be approximately constant as $\ell \to L$, ensuring that $\mathcal{F}_\ell$ is a good enough approximation even on the coarsest level $\ell = 0$. Furthermore, $\mathbb{V}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ and $\mathbb{E}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ should decay rapidly as $\ell \to L$, ensuring that the approximation error decreases with increasing level. $\mathbb{V}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ may be expanded as

$$\mathbb{V}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}] = \mathbb{V}[\mathcal{F}_\ell] + \mathbb{V}[\mathcal{F}_{\ell-1}] - 2 \cdot \mathrm{Cov}(\mathcal{F}_\ell, \mathcal{F}_{\ell-1}), \tag{5}$$

showing that it should be given that $2 \cdot \mathrm{Cov}(\mathcal{F}_\ell, \mathcal{F}_{\ell-1}) > \mathbb{V}[\mathcal{F}_{\ell-1}]$, which requires $\mathcal{F}_\ell$ and $\mathcal{F}_{\ell-1}$ to be sufficiently correlated.

While those relations between levels are not formally required to hold for inversion, they ensure that the multilevel estimator for the expectation of $\mathbf{Y}$ has reduced variance and is computationally more efficient compared to a single-level estimator (Cliffe et al., 2011; Lykkegaard et al., 2023). While a deviation of the previously described optimal relations between levels does not necessarily indicate a poorly performing model hierarchy, without such a deviation the hierarchy may be said to be well behaved.

During multilevel inversion, no explicit approach exists yet to pre-define (or optimize) the number of levels or the refinement (or coarsening, respectively). Dodwell et al. (2019); Lykkegaard et al. (2023) arbitrarily pre-define the coarsening as well as the number of levels considered but give some analysis of the effect regarding the number of levels. In similar examples to our subsequently considered benchmark example of groundwater flow, Cliffe et al. (2011) consider 5 levels, Dodwell et al. (2019) consider up to 5 levels, Lykkegaard and Dodwell (2022) consider 2 levels, and Lykkegaard et al. (2023) consider 3 levels.

2.2 Multilevel Markov-chain Monte Carlo

The multilevel delayed acceptance (MLDA) MCMC algorithm was developed by Lykkegaard et al. (2023) on the basis of the delayed acceptance algorithm coupled with the randomized-length-subchain surrogate transition (Christen & Fox, 2005; J. S. Liu, 2008). The main functionality of MLDA is shown in Fig. 1 for a case with two levels. We use the Python implementation of MLDA by Lykkegaard (2022) with fixed-length subchains and the option of running a number of n_{chains} chains in parallel. In the re-

mainder we also assume that the parameter vectors $\{\boldsymbol{\theta}_\ell\}_{\ell=0}^{L}$ are comprised of the same model parameters, i.e., we do not consider level-dependent or different coarse and fine (or nested) model parameter vectors.

While other MCMC algorithms sample from a single (posterior) distribution as given in Eq. 2, MLDA considers a hierarchy of distributions $p_0(\cdot), \ldots, p_\ell(\cdot), \ldots, p_L(\cdot)$ that are computationally cheap approximations of the target density $p(\cdot)$, where each $p_\ell(\cdot)$ may be defined according to Eq. 2 corresponding to each model in $\{\mathcal{F}_\ell\}_{\ell=0}^{L}$. The MLDA algorithm then gets called on the highest level density $p_L(\cdot)$. By recusively calling the MLDA algorithm on level $\ell - 1$, subchains with length J_ℓ are generated on levels $1 \leq \ell \leq L$ until level $\ell = 0$ is reached. We note that different subchain lengths may be used on different levels but the analysis here is restricted to the same $J_\ell = J$ on all levels. On the lowest level $\ell = 0$, a conventional MCMC sampler is invoked. The final state of a subchain on level $\ell - 1$, $\boldsymbol{\theta}_{\ell-1}^{J_\ell}$, is finally passed as a proposal to the higher-level chain on level ℓ. Subsequently, only samples from the highest level are considered for inference. A conventional single-level MCMC sampler may be obtained with using MLDA if only the highest-level model is considered. We note that for MLDA the relation between different levels is not formally required to show decaying variance and mean as described in section 2.1.

As with any MCMC algorithm, MLDA posterior uncertainty estimates for (highest-level) model outputs may be computed as confidence intervals from simulations made with posterior samples, which are obtained during sampling. MCMC (and MLDA) samples are naturally correlated and may show dependence on initial samples, requiring that an initial number of samples are burned and that that samples are thinned (e.g., every other sample may be omitted to reduce autocorrelation) (e.g., Vrugt, 2016; Lykkegaard et al., 2023). To assess convergence of the Markov-chains, the Gelman-Rubin statistic $\widehat{R}$ is frequently used for multi-chain samplers (Gelman & Rubin, 1992). A value of $\widehat{R} \leq 1.2$ is often deemed sufficient to ensure convergence (e.g., Vrugt, 2016).

2.3 Multilevel Generalized Likelihood Uncertainty Estimation

The Generalized Likelihood Uncertainty Estimation (GLUE) methodology rejects the formal (Bayesian) statistical basis of inference and instead seeks to identify a set of system representations (combinations of model inputs, model structures, model parameters, model errors) that are sufficiently consistent with the observations of that system (Beven & Freer, 2001; Vrugt et al., 2009; Beven & Binley, 2014; Mirzaei et al., 2015). In the GLUE methodology the models used for inference are not considered to be true, contrary to the case of formal Bayesian inversion.

The likelihood function in GLUE aggregates all aspects of error and consistency as a generalized fuzzy belief. It serves as a decision threshold to separate behavioural (i.e., good agreement between $\mathbf{Y}$ and $\widetilde{\mathbf{Y}}$) and non-behavioural (i.e., poor agreement between $\mathbf{Y}$ and $\widetilde{\mathbf{Y}}$) simulations. Beven and Binley (1992) and (Beven & Freer, 2001) introduced a number of different functions for this purpose and the following likelihood

is frequently used (Vrugt et al., 2009):

$$\widetilde{\mathcal{L}}(\boldsymbol{\theta}|\widetilde{\mathbf{Y}}) := (\sigma_r^2)^{-T} = \left(\frac{\sum_{i=1}^{k} (y_i - \tilde{y}_i)^2}{k-2} \right)^{-T} \tag{6}$$

Parameter and model output uncertainty is estimated in GLUE by running the model with N parameter samples randomly drawn from the prior distribution $\{\boldsymbol{\theta}^{(j)}\}_{j=1}^{N}$ and evaluating the likelihood function for each sample. The likelihood threshold may either be defined a-priori (as a certain value above which a model realization is considered behavioural) or may be defined as a percentage based on the set of all likelihood corresponding to the evaluated parameter samples (by setting the threshold to, e.g., the top 10% of the likelihood values) (Beven & Binley, 1992; Beven & Freer, 2001; Vrugt et al., 2009). Using only behavioural solutions, (cumulative) probability distributions of model outputs are generated, from which uncertainty estimates are finally computed. Behavioural parameter samples are used to estimate the posterior distribution of model parameters.

MLGLUE is generally similar to MLDA (or MLMCMC) as shown in Fig. 1. As with MLDA, a parameter sample $\boldsymbol{\theta}^{(j)}$ is only finally accepted if it is accepted on the highest level. While MLDA makes use of an acceptance probability on all levels (as it is typical in MCMC algorithms), MLGLUE uses a level-dependent likelihood threshold on all levels to distinguish between samples being accepted (i.e., behavioural solutions) and samples being discarded (i.e., non-behavioural solutions).

MLGLUE requires that likelihood thresholds are available for every level prior to sampling. While pre-defined likelihood thresholds can optionally be used, MLGLUE implements the estimation of the likelihood thresholds via Monte Carlo sampling, where an identical set of parameter samples is evaluated on each level. We refer to that as *tuning* and the number of tuning samples in that set, N_t, should be substantially smaller than the overall number of samples being evaluated with MLGLUE, $N_t \ll N$. Calculating corresponding likelihood values for each of those tuning samples then results in an individual set of likelihood values for each level. We denote the set of likelihood samples on a single level by $\{\widetilde{\mathcal{L}}^{(i,\ell)}\}_{i=1}^{N_t}$ and the combined set for all levels by $\{\{\widetilde{\mathcal{L}}^{(i,\ell)}\}_{i=1}^{N_t}\}_{\ell=0}^{L}$. From those sets the likelihood threshold is calculated for each level as a pre-defined percentage; we denote the set of likelihood thresholds on each level by $\{\widetilde{\mathcal{L}}_{T,\ell}\}_{\ell=0}^{L}$.

From the set of likelihood values on each level, $\{\{\widetilde{\mathcal{L}}^{(i,\ell)}\}_{i=1}^{N_t}\}_{\ell=0}^{L}$, sample estimates of $\mathbb{V}[\widetilde{\mathcal{L}}_\ell]$, $\mathbb{E}[\widetilde{\mathcal{L}}_\ell]$, $\mathbb{V}[\widetilde{\mathcal{L}}_\ell - \widetilde{\mathcal{L}}_{\ell-1}]$, and $\mathbb{E}[\widetilde{\mathcal{L}}_\ell - \widetilde{\mathcal{L}}_{\ell-1}]$ for $\ell = 0, \ldots, L$ are computed to analyze the relation between levels regarding the likelihood.

Afterwards, *sampling* is started and parameter samples $\boldsymbol{\theta}^{(j)}$ are initially evaluated with the model on level $\ell = 0$. If the corresponding likelihood is greater or equal to the level-dependent threshold, the sample is passed to the next higher level and is evaluated again. This process is repeated until the highest level is reached and the sample is finally considered behavioural or non-behavioural. If the likelihood is smaller than the level-dependent threshold on any level, the sample is immediately regarded as non-behavioural and the next sample is considered. Therefore, samples with low likelihood are disregarded

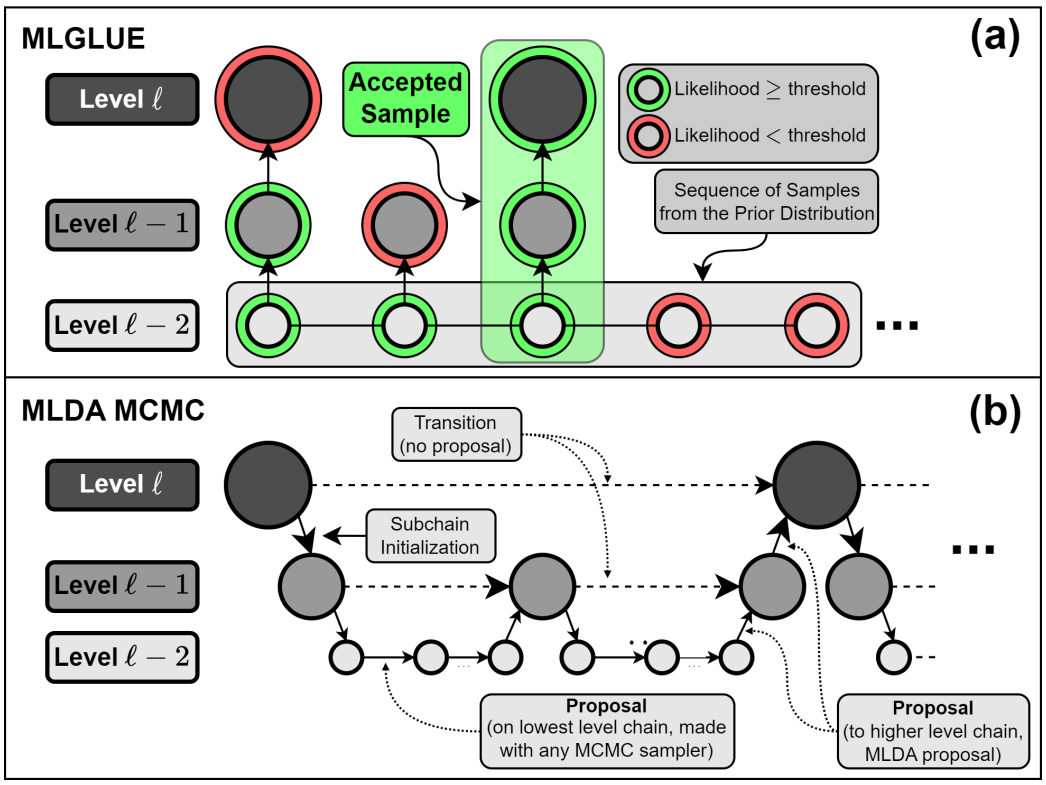

Figure 1. Schematic representation of multilevel sampling strategies for the case of three levels; (a) MLGLUE approach, green rings indicate a likelihood that is above the level-dependent threshold, red rings indicate the contrary; (b) Multilevel Delayed Acceptance MCMC; circles represent the state or current parameter sample

already on lower levels, leading to substantial computational savings. In the supporting information, the reasoning for using level-dependent likelihood thresholds as well as the structure of the algorithm is clarified in more detail.

The MLGLUE algorithm is shown in Fig. 2 and involves the following steps during sampling (tuning is excluded here):

1. Draw a sample $\boldsymbol{\Theta}_0$ of N points from the (typically uniform) prior distribution $p_p(\boldsymbol{\theta})$ and set $j = 0$
2. Set $\ell = 0$ and
   (a) Compute the likelihood $\widetilde{\mathcal{L}}^{(j,\ell)} = \widetilde{\mathcal{L}}(\boldsymbol{\theta}^{(j)}|\widetilde{\mathbf{Y}})$ with sample $\boldsymbol{\theta}^{(j)}$ from $\boldsymbol{\Theta}_0$ and with the model on level ℓ
      i. if $\ell = L$ and $\widetilde{\mathcal{L}}^{(j,\ell)} \geq \widetilde{\mathcal{L}}_{T,\ell}$, store $\boldsymbol{\theta}^{(j)}$ in matrix $\mathbf{B}$, increment $j \leftarrow j + 1$, and go back to step 2
      ii. if $\widetilde{\mathcal{L}}^{(j,\ell)} \geq \widetilde{\mathcal{L}}_{T,\ell}$, increment $\ell \leftarrow \ell + 1$ and go back to step 2a
      iii. if $\widetilde{\mathcal{L}}^{(j,\ell)} < \widetilde{\mathcal{L}}_{T,\ell}$, increment $j \leftarrow j + 1$ and go back to step 2

iv. if $j = N$, break the iteration and go to step 3

3. For each $i = 1, \ldots, N_b$ in $\mathbf{B}$, normalize the corresponding likelihood via $\widetilde{\mathcal{L}}'(\mathbf{B}^{(i)}|\widetilde{\mathbf{Y}}) = \widetilde{\mathcal{L}}(\mathbf{B}^{(i)}|\widetilde{\mathbf{Y}}) / \sum_{i'=1}^{N_b} \widetilde{\mathcal{L}}(\mathbf{B}^{(i')}|\widetilde{\mathbf{Y}})$
4. For each $\mathbf{Y}^i, i = 1, \ldots, N_b$ in $\mathbf{B}$, assign the corresponding probability $\widetilde{\mathcal{L}}'(\mathbf{B}^{(i)}|\widetilde{\mathbf{Y}})$
5. Sort the $\mathbf{Y}^i, i = 1, \ldots, N_b$ increasingly according to their probability and create uncertainty intervals from the obtained distribution

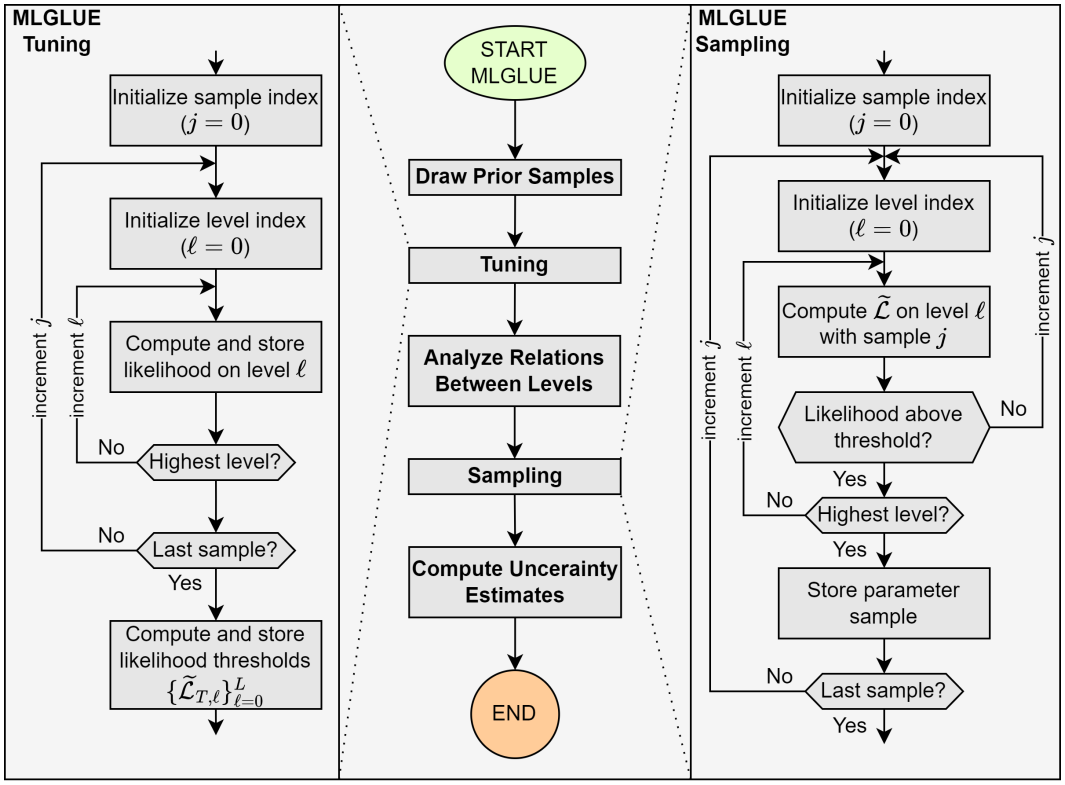

Figure 2. Schematic representation of the multilevel Generalized Likelihood Uncertainty Estimation algorithm; tuning refers to the (optional) Monte Carlo estimation of likelihood thresholds, sampling refers to the repeated evaluation of parameter samples (see the description of algorithm steps)

2.4 Convergence Analysis

Although the Gelman-Rubin statistic (see section 2.2) is widely used to assess convergence of MCMC chains, the statistic is restricted to multi-chain methods. Because MLGLUE and GLUE do not operate with multiple chains, we introduce an alternative methodology to assess convergence.

Let $\mathbf{B}$ be the $N \times n$ matrix of samples, where an individual row or column is indexed as $\mathbf{B}_{i,*}$ or $\mathbf{B}_{*,j}$, respectively. The normalized relative deviation $\mathcal{D}$ of a sub-sample

of $\mathbf{B}$, having length i, from the global mean of the corresponding j-th parameter in $\mathbf{B}$ is then computed as

$$\mathcal{D}_{i,j} = \frac{\frac{1}{i}\sum_{k=1}^{i} \mathbf{B}_{k,j}}{\frac{1}{N}\sum_{k=1}^{N} \mathbf{B}_{k,j}} - 1 \tag{7}$$

Assessing convergence for all possible i results in a sequence of relative deviations $\{\mathcal{D}_{i,j}\}_{i=1}^{N}$ for a parameter j. Bootstrap replicates of $\mathcal{D}_{i,j}$ for each i are then computed, resulting in average normalized relative deviations from the global mean $\widehat{\mathcal{D}}_{i,j}$. Convergence is assumed when $\widehat{\mathcal{D}}_{i,j}$ continuously stays within a pre-defined tolerance range (e.g., ± 0.05). Analyzing after which fraction of N $\widehat{\mathcal{D}}_{i,j}$ continuously stays within a tolerance range (e.g., ± 0.05) furthermore enables the assessment of convergence behaviour.

2.5 Test Problems

The test problems discussed in sections 2.5.1 and 2.5.2 are used to show the differences between the methods of statistical inference (MLGLUE, GLUE, MLDA, MCMC) regarding obtained posterior distributions, uncertainty estimates for model output, and computational efficiency. An identical number of prior parameter samples is used for all methods to ensure comparability. For GLUE and MLGLUE, an informal (Eq. 6) as well as a formal (Eq. 3) likelihood function are used for each problem. MCMC and MLDA are used with a formal likelihood function (Eq. 3). Gaussian (iid) random noise is added to each set of observations, making the assumptions for defining Eq. 3 valid.

The same number of CPUs as well as the same framework for parallelization are used for all methods. For reasons of reproducibility, seeds are used for pseudo-random number generation, which is used in multiple places (e.g., drawing samples form a distribution); the same seeds are used for all methods of inference in the example under study.

All methods of inference are implemented in the `Python` programming language. The `tinyDA v0.9.8` (Lykkegaard, 2022) package is used for MLDA and MCMC sampling with a DREAM(Z)-sampler, which is similar to the DREAM(ZS)-sampler (Vrugt, 2016; Lykkegaard, 2022), using `Ray v2.2.0` (Team, 2022) for parallelization. `ArviZ v0.12.1` (Kumar et al., 2019) is used for the analysis of MLDA and MCMC results (convergence, effective sample size); in `tinyDA`, the initial sample is returned additionally to the N. MLGLUE is implemented as a `Python` package and also enabled for parallel computing with `Ray v2.2.0` (Team, 2022).

2.5.1 Linear Regression

The first case study is a simple linear equation in one dimension:

$$f(\boldsymbol{\theta}) = \boldsymbol{\theta}_1 x + \boldsymbol{\theta}_2, \quad x \in [0, 1] \tag{8}$$

$$\widetilde{\mathbf{Y}} = f(\boldsymbol{\theta}) + \mathcal{N}(\mu = 0, \sigma = 0.8) \tag{9}$$

where θ_1 represents the slope and θ_2 represents the intercept; $\boldsymbol{\theta} = [\theta_1, \theta_2]^T$. A total of $n = 500$ samples are obtained, forming $\widetilde{\mathbf{Y}}$, by calculating $\mathcal{F}(\boldsymbol{\theta})$ for 500 linearly spaces points $x \in [0, 1]$ with $\theta_1 = 2$ and $\theta_2 = 1$. The true model as well as noisy observations are shown in Fig. 3.

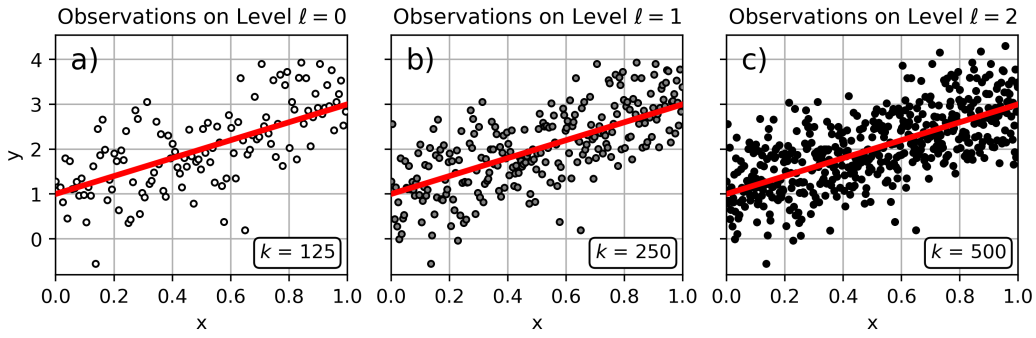

Figure 3. True model (red line) as well as noisy observations on levels $\ell = 0$ (a), $\ell = 1$ (b), and $\ell = 2$ (c) for the regression example

Eq. 8 does not need to be discretized as it is a closed-form expression for the system response. Similar to the linear regression example from Lykkegaard (2022), the different levels are obtained by considering all observations for the highest level and subsequently removing observations to represent lower levels. We chose the total number of levels to be 3, i.e., $\ell = 0, 1, 2$, where all 500 observations are considered on level $\ell = 2$, every second observation is considered on level $\ell = 1$, and every fourth observation is considered on level $\ell = 0$. The different sets of observations are represented in Fig. 3.

The prior distribution $p_0(\boldsymbol{\theta})$ is chosen to be a uniform distribution with lower bounds $\theta_{1,l} = -4$ and $\theta_{2,l} = -2$ and upper bounds $\theta_{1,u} = 4$ and $\theta_{2,u} = 2$. A total number of $N_t + N = 2,000 + 98,000 = 100,000$ samples are drawn from $p_p(\boldsymbol{\theta})$ with each inference method, where $N_t = 2,000$ samples are used to estimate the level-dependent likelihood thresholds (see section 2.3) and to analyze the relations between the levels (see section 2.1) in MLGLUE. A constant variance equal to the constant additive Gaussian noise variance ($\sigma^2 = 0.8$) is used for the Gaussian likelihood (see Eq. 3); for informal likelihoods (see Eq. 6) $T = 1$ is used. The likelihood thresholds are estimated to correspond to the best 0.2% of simulations. For MLDA, the sub-sampling rate is set to 5. All methods are run on 5 CPUs.

We note that both likelihood functions used are dependent on the number of observations considered. With the sum of squared residuals, data variance, and error variance held constant, the likelihood in Eq. 6 will increase while the likelihood in Eq. 3 will decrease with an increasing number of observations. Because a different number of observations is used on different levels in the present problem, this effect weakens the ex-

planatory power of the relations between levels (see section 2.1) shown in Fig. 5 (and in Fig. S1 in the supporting information). This is due to the fact that those opposing dependencies on the number of observations greatly superimpose the effects of the sum of suqared residuals on the likelihood when going from ℓ to $\ell + 1$.

2.5.2 Groundwater Flow

The second example considers steady-state two-dimensional groundwater flow in an aquifer with inhomogeneous horizontal hydraulic conductivity, Dirichlet-type (fixed potentials), Neumann-type (no-flow conditions, recharge), Robin-type (river), and nodal sink type (wells) boundary conditions:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) + R = 0 \tag{10}$$

$$h = h_c \quad \forall y \in \partial\Omega, x = 0\ m \tag{11}$$

$$\frac{\partial h}{\partial y} = 0 \quad \forall x \in \partial\Omega, y \in \{0\ m, 5,000\ m\} \tag{12}$$

$$\frac{\partial h}{\partial x} = 0 \quad \forall y \in \partial\Omega, x = 10,000\ m \tag{13}$$

$$f_{riv} = c_{riv}\Delta h \quad \forall 0\ m \leq x \leq 10,000\ m, y = 1,000\ m \tag{14}$$

where K $[LT^{-1}]$ is the hydraulic conductivity field, h $[L]$ is the hydraulic head field, R $[LT^{-1}]$ is the recharge flux, f_{riv} $[LT^{-1}]$ is river inflow, and c_{riv} $[T^{-1}]$ is riverbed conductance. The model is set up with the finite-differences code `MODFLOW-NWT` and the reader is referred to Harbaugh (2005) and Niswonger et al. (2011) for a detailed description of the model and boundary condition implementations.

The reference model is discretized as a regular structured grid with a cell-size of 25 $m \times 25$ m, having 200 rows and 400 columns. The aquifer bottom is horizontal at 10.0 m above the reference datum; the aquifer top represents a tilted plane falling linearly from 50.0 m on the left side of the domain to 40 m above the reference datum on the right side of the domain. A river crosses the domain along a single row, having a constant water level at 1.0 m below the aquifer top and a river bottom at 4.0 m below the aquifer top. 5 wells are placed in the model domain with a total extraction rate of 700 md^{-1}. Spatially uniform recharge is applied with a rate of $2 \cdot 10^{-5}$ md^{-1}. A constant head of 45.0 m above the reference datum is assigned to the leftmost column of cells. 12 observation points as well as 1 prediction point are placed in the domain.

The hydraulic conductivity in every cell is obtained in the reference model using a regular grid of pilot points (e.g., Doherty, 2003), linearly spaced (5 along columns, 10 along rows) starting on the domain boundaries. Reference values of pilot point hydraulic conductivities are obtained by sampling from a log-normal distribution with $\mu = 0.3$ and $\sigma = 0.7$. Gaussian process regression (GPR), as implemented in `scikit-learn v1.2.0` (Pedregosa et al., 2011), is used to interpolate hydraulic conductivities at cell centers of the reference model with a radial basis function kernel with a fixed length scale of 600 m.

The model domain and its main characteristics are shown in Fig. 4 for the models on levels $\ell = 0$ and $\ell = 3$.

The reference model is also the highest-level model. Besides this model, three lower-level models are considered, resulting in $\ell = 0, 1, 2, 3$. Lower-level models are obtained via grid coarsening, where cell sizes are doubled going from ℓ to $\ell-1$. Lower-level hydraulic conductivity values at each cell are obtained by using the geometric mean of corresponding higher-level cells.

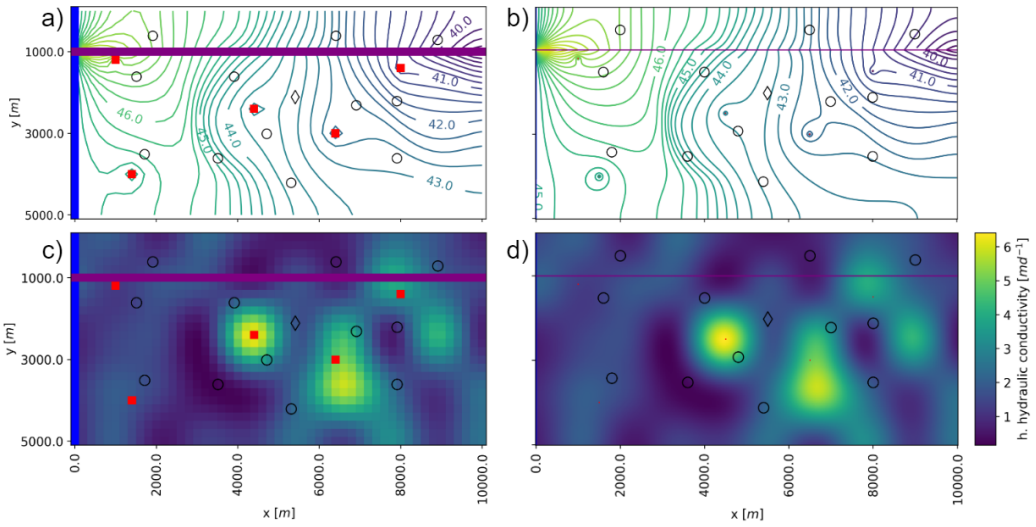

Figure 4. Groundwater flow model domain; head contours obtained with true parameters on level $\ell = 0$ (a) and on level $\ell = 3$ (b); horizontal hydraulic conductivity field on level $\ell = 0$ (c) and on level $\ell = 3$ (d); specific characteristics are: constant head cells (blue), river cells (purple), wells (red), observation points (circles), prediction point (diamond)

Besides the 50 pilot point parameters, the GPR length scale is considered a model parameter as well; $\boldsymbol{\theta} = [\theta_{1,PP}, \ldots, \theta_{50,PP}, \theta_{51,GPR}]^T$. We denote the parameter-to-observable map (i.e., Eqs. 10 to 14) by $\mathcal{M}(\boldsymbol{\theta})$. Adding Gaussian random noise to the observations then leads to $\widetilde{\mathbf{Y}} = \mathcal{M}(\boldsymbol{\theta}) + \mathcal{N}(\mu = 0, \sigma = 1)$.

As a prior distribution $p_p(\boldsymbol{\theta})$, a uniform distribution is chosen with lower bounds $\boldsymbol{\theta}_l = [1 \cdot 10^{-2}, \ldots, 1 \cdot 10^{-2}, 5 \cdot 10^{2}]$ and upper bounds $\boldsymbol{\theta}_u = [1 \cdot 10^{1}, \ldots, 1 \cdot 10^{1}, 1 \cdot 10^{3}]$. A total number of $N_t + N = 2,000 + 98,000 = 100,000$ samples are drawn from $p_0(\boldsymbol{\theta})$ with each inference method, where $N_t = 2,000$ samples are used to estimate the level-dependent likelihood thresholds (see section 2.3) and to analyze the relations between the levels (see section 2.1) in MLGLUE. A constant variance equal to the constant additive Gaussian noise variance ($\sigma^2 = 0.8$) is used for the Gaussian likelihood (see Eq. 3); for informal likelihoods (see Eq. 6) $T = 1$ is used. The likelihood thresholds are es-

timated to correspond to the best 2% of all simulations. For MLDA, the sub-sampling rate is set to 5. All methods are run on 50 CPUs.

3 Results and Discussion

For the two examples considered, we now present results of inversion with the methodologies of MLGLUE, GLUE, MLDA, and MCMC. We analyze how models on different levels are related (i.e., for MLGLUE and MLDA) and how the results obtained with a multilevel approach differ from the conventional approach using a single model. Differences between the different methods are discussed regarding obtained posterior distributions, uncertainty estimates for model output, and computational efficiency. Results of convergence analysis are given in the supporting information.

The resulting uncertainty estimates, parameter posterior distributions, and convergence behaviour are virtually identical when using either formal or informal likelihood functions in GLUE and MLGLUE. Therefore, the corresponding results are discussed with a focus on using an informal likelihood function in this section. Results from GLUE and MLGLUE using a formal likelihood are mainly given in the supporting information for both example problems.

MCMC chains typically exhibit a transition period where the samples approach the posterior distribution. The samples of this transition period are discarded as *burn-in* (Gallagher et al., 2009; Brunetti et al., 2023). GLUE and MLGLUE both result in independent posterior samples, while MCMC and MLDA result in correlated posterior samples. To compare both groups (GLUE & MLGLUE and MCMC & MLDA) on an equal basis, independent samples are obtained from MCMC and MLDA samples via *thinning*; only every $\mathcal{K}$-th sample is considered for subsequent analysis. We apply thinning such that the thinned number of samples is approximately equal to the estimated effective sample size of unthinned samples.

3.1 Linear Regression

This example considers the problem of estimating the parameters of slope and intercept from noisy observations of a one-dimensional linear regression model. Subsets of different size of the observed data are used on the different model levels instead of utilizing models with different spatial or temporal discretization. After analyzing the relation between the models on different levels, we assess the quality of inferences made with MLGLUE compared to other methods.

The relations between the three levels are shown in Fig. 5, from which it is apparent that $\mathbb{V}[\mathcal{F}_\ell]$ and $\mathbb{E}[\mathcal{F}_\ell]$ are approximately constant and that that $\mathbb{V}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ and $\mathbb{E}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ decay across all levels. Therefore, the approximation error of the likelihoods apparently decreases in the informal case as $\ell \to L$, although this effect is superimposed by the influence of different numbers of obervations on the likelihood.

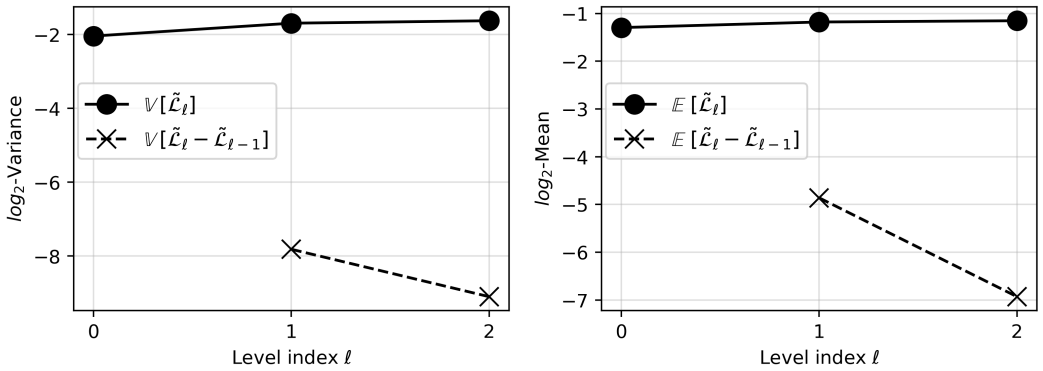

Figure 5. Relations between levels for the linear regression example, using an informal likelihood

The sampling efficiencies of all methods are shown in Tab. 1, showing that the number of effective samples is comparable for all methods of inference. The MLDA and MCMC computation time exceeds that of MLGLUE and GLUE by a factor ≥ 4. GLUE is associated with the highest number of effective samples per minute, followed by MLGLUE, MCMC, and MLDA. Taking the low computational cost of a single model run into account, the differences in computation time can be attributed to different computational complexities of the algorithms. We also note that the initialization time of the parallelization framework dominates the overall computation times; without parallelization, the computation time is approximately one order of magnitude smaller. This effect, however, diminishes when the computational cost of a single model call increases.

Table 1. Sampling efficiency for the linear regression example

Method	Time	No. of calls on $\ell = 2$	No. of Posterior Samples	No. of Effective Post. Samples	Effective Samples per Minute
MLGLUE (I)[a]	23 s	582	300	300	782.6
MLGLUE (F)[b]	25 s	582	300	300	720.0
GLUE (I)[a]	23 s	100,000	344	344	897.4
GLUE (F)[b]	22 s	100,000	344	344	938.2
MLDA	109 s	4,000	4,000	289	159.1
MCMC	100 s	100,000	100,000	385	231.0

[a]Informal likelihood

[b]Formal likelihood

For each of the two parameters, MLGLUE and GLUE converge similarly quickly, followed by MLDA and MCMC. More detailed results of convergence analysis are shown in the supporting information.

Kernel density estimates of the parameter posteriors are shown in Fig. 6 (a) and (b). Posteriors for MLGLUE and GLUE are more heavy-tailed and have a smaller span, or variance, compared to the MLDA and MCMC posteriors. The distribution median is closest to the true values for both parameters for MLGLUE, followed by GLUE, MCMC, and MLDA. The more heavy-tailed posteriors of MLGLUE and GLUE may be attributed to the equifinality concept inherent to the GLUE methodology (Beven, 1993; Vrugt et al., 2009) and to the pre-defined threshold, which effectively controls the number of (effective) samples as well as the distribution variance. Small deviations in slope and intercept parameters would still result in a high likelihood, which would be considered behavioural with the GLUE methodology. We note that MLGLUE posterior samples are equal regardless of using a formal or an informal likelihood function. All posterior samples from MLGLUE are furthermore reflected in GLUE posterior samples, which are also equal using either a formal or an informal likelihood function. 44 GLUE posterior samples are not in the MLGLUE posterior samples, which can be attributed to the samples being discarded on lower levels in MLGLUE. Those sample differences are reflected in the different span and tails of the distributions.

Uncertianty estimates obtained from simulated values corresponding to posterior parameter samples are shown in Fig. 6. The estimates are generally similar for all methods of inference, however GLUE as well as MLDA and MCMC median estimates are initially more biased towards higher values than MLGLUE estimates. Coefficients of determination computed for median simulation and true values are virtually equal for all methods of inference. This result is in agreement with the findings of (Vrugt et al., 2009), where different posteriors from formal Bayesian inversion with MCMC and informal results from GLUE would still result in similar uncertainty estimates of simulated values.

3.2 Groundwater Flow

This example considers the estimation of pilot point hydraulic conductivity values along with the length scale parameter of a Gaussian process. Four models with decreasing spatial resolution are considered during multilevel inversion. We analyze the relations between the models on different levels, assess the quality of inferences made with MLGLUE compared to other methods of inference, and quantify computational efficiency.

The relations between the three levels are shown in Figs. 7, from which it is apparent that $\mathbb{V}[\mathcal{F}_\ell]$ and $\mathbb{E}[\mathcal{F}_\ell]$ are approximately constant and that that $\mathbb{V}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ and $\mathbb{E}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ decay across all levels when using the likelihood function Eq. 6. The variance of the sampled likelihoods on level $\ell = 0$, however, is smaller than on higher levels.

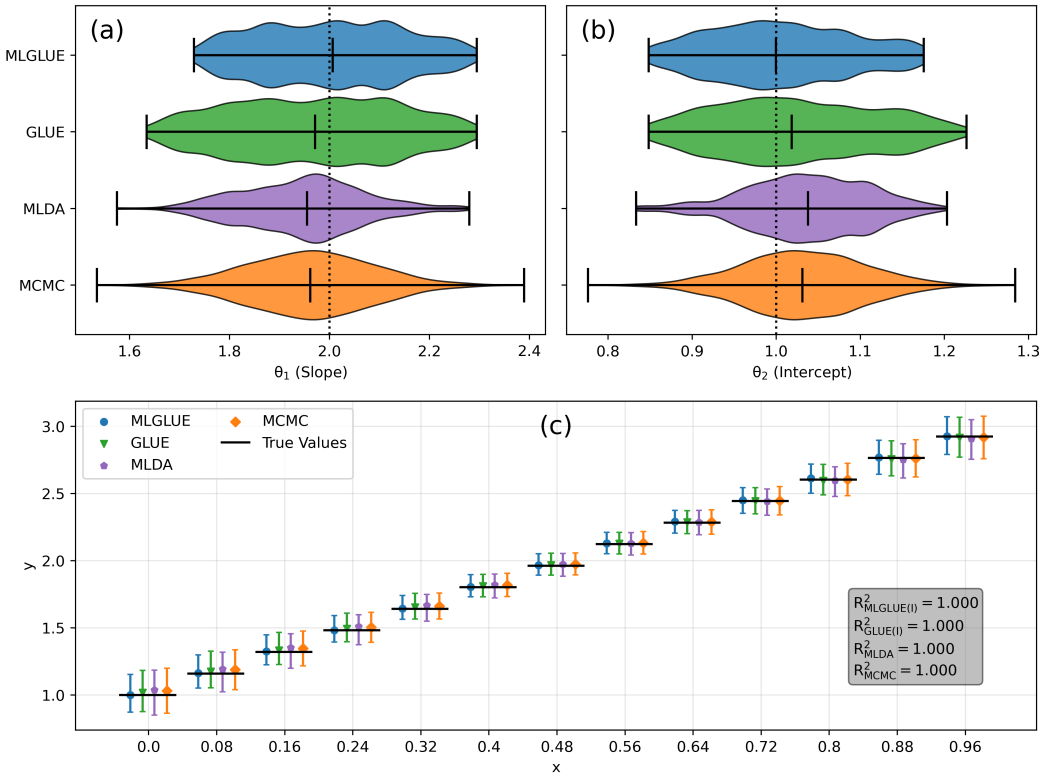

Figure 6. Kernel density estimates of model parameters, where solid vertical lines represent distribution median values and dashed lines represent the true parameter values (a, b) and $99\% - 1\%$ uncertainty estimates around the median value (c)

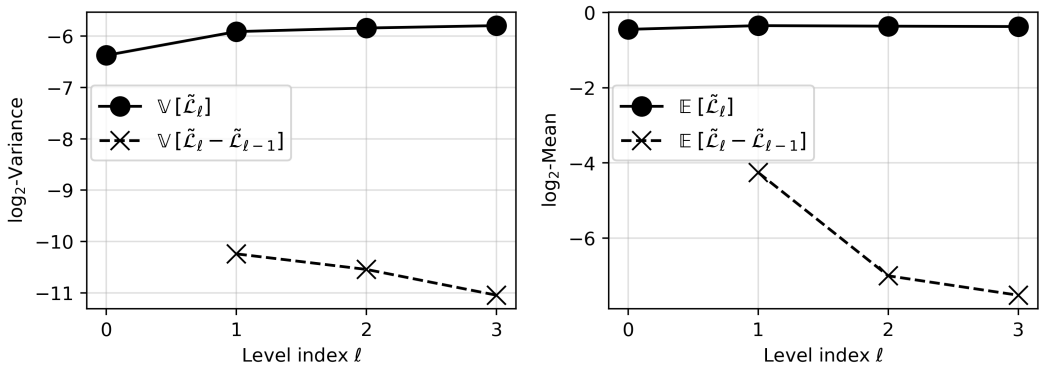

Figure 7. Relations between levels for the groundwater flow example, using an informal definition of the likelihood

The sampling efficiencies of all methods are shown in Tab. 2, showing that the number of effective samples is comparable for all methods of inference. The computation times of single-level inference (i.e., GLUE with informal and formal likelihood and MCMC) and of multilevel inference (i.e., MLGLUE with informal and formal likelihood and MLDA)

are similar, respectively; the computation time of single-level inference exceeds that of multilevel inference by a factor of ≈ 2. MLGLUE is associated with the highest number of effective samples per minute, followed by GLUE, MLDA, and MCMC. This example clearly shows the benefit of using multilevel methods for inference, as overall computation times can be substantially reduced compared to single-level methods.

Table 2. Sampling efficiency for the groundwater flow example

Method	Time	No. of calls on $\ell = 3$	No. of Posterior Samples	No. of Effective Post. Samples	Effective Samples per Minute
MLGLUE (I)[a]	$1,992\ s$	$1,915$	331	331	10.0
MLGLUE (F)[b]	$1,906\ s$	$1,917$	333	333	10.5
GLUE (I)[a]	$3,670\ s$	$100,000$	398	398	6.5
GLUE (F)[b]	$3,415\ s$	$100,000$	398	398	7.0
MLDA	$2,052\ s$	800	800	267	7.8
MCMC	$4,671\ s$	$100,000$	$100,000$	385	4.9

[a]Informal likelihood

[b]Formal likelihood

Averaged over all pilot point parameters, GLUE converges more quickly than MCMC, followed by MLGLUE and MLDA. However, MCMC samples converge more rapidly compared to MLGLUE, GLUE, and MLDA for the length scale parameter. More detailed results of convergence analysis are shown in the supporting information.

Kernel density estimates of the parameter posteriors are shown in Fig. 8 (a) - (d). Often, as for PP No. 3 or PP No. 38, MLGLUE and GLUE posteriors are substantially more heavy-tailed than their MLDA and MCMC counterparts. The absolute deviation of estimated posterior median values from true parameter values, averaged over all 50 PP parameters, is 3.43, 3.42, 3.38, and 3.30 for MLGLUE, GLUE, MLDA, and MCMC, respectively. The equifinality concept in the GLUE methodology (Beven, 1993; Vrugt et al., 2009) manifests itself in the corresponding posterior distributions to be more heavy-tailed. The variance of the posterior distributions is furthermore controlled by the predefined likelihood threshold. Deviations in PP hydraulic conductivity values - in combination with a different GPR length scale - would still result in similar hydraulic conductivity fields, which is directly reflected in the more heavy-tailed MLGLUE and GLUE posteriors. PP parameters near observations points, however, are substantially more informed by the data, decreasing the distribution variance in MLGLUE and GLUE (see Fig. 8 (b)). MLGLUE posterior samples are highly similar regardless of using formal or informal likelihood functions, where only two additional samples are considered behavioural when using a formal likelihood function. All posterior samples from MLGLUE are fur-

thermore reflected in GLUE posterior samples, which are exactly equal with a formal or informal likelihood function. Several GLUE posterior samples are not in the MLGLUE posterior samples, which can be attributed to the samples being discarded on lower levels with MLGLUE. Those sample differences are reflected in the different span and tails of the posteriors, which are, however, very similar.

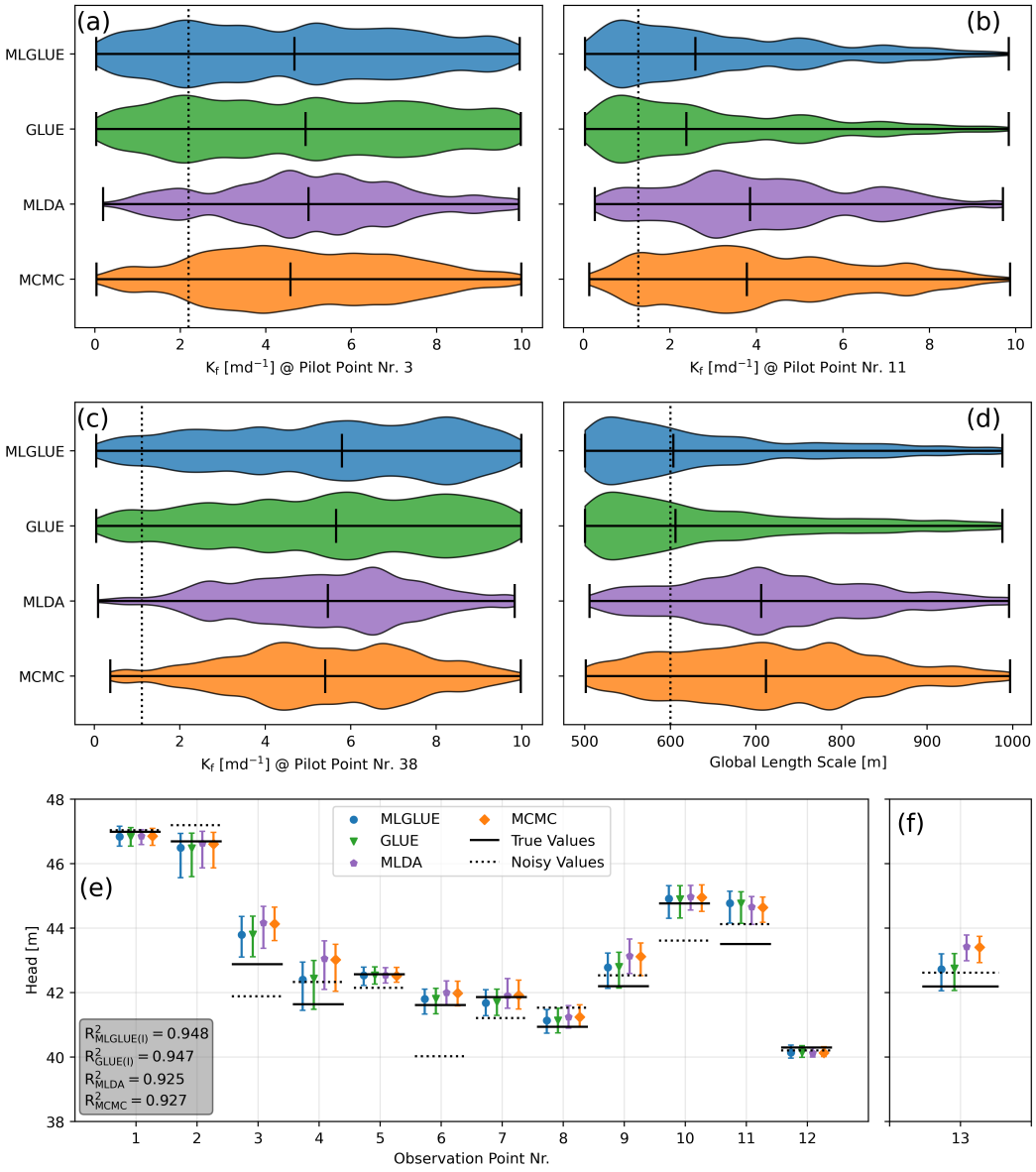

Figure 8. Kernel density estimates of model parameters, where solid vertical lines represent distribution median values and dashed lines represent the true parameter values (a, b, c, d) and 99% – 1% uncertainty estimates around the median value for observation points (e) and for the prediction point(f)

Uncertainty estimates obtained from simulated values corresponding to posterior parameter samples are shown in Fig. 8. For observation points 1, 2, 5, 8, 10, 11, and 12, the uncertainty estimates and median values are generally similar for all methods of inference. For all other observation points as well as for the prediction point, uncertainty estimates and median values from MLGLUE and GLUE reflect the true values better than the MLDA and MCMC counterparts. This is also reflected in the coefficients of determination computed for median simulation and true values. They are virtually equal for MLGLUE and GLUE methods and lower values were observed for MLDA and MCMC. This result is in partial agreement to the findings of (Vrugt et al., 2009), where different posteriors from formal Bayesian inversion with MCMC and informal results from GLUE still resulted in similar uncertainty estimates of simulated values. For multiple observation points, however, MLDA and MCMC estimates more strongly deviate from MLGLUE and GLUE results. This can not only be attributed to the likelihood function used (as the same likelihood function is used in the cases of formal MLGLUE and GLUE as well as MLDA and MCMC) but also to the general approaches of a Monte Carlo type (MLGLUE and GLUE) and Markov-chain Monte-Carlo type (MLDA and MCMC); MCMC-type inferences are often over-confident, especially when using uninformative prior distributions (Gelman et al., 2021).

4 Conclusions

In hydrological sciences, the popularity of statistical inference and inversion has remained high in recent years. However, the applicability of corresponding approaches to more complex models and in the context of digital twins has been limited by the associated computational cost when solving inverse problems. The goal of our study is to introduce and test an extension to the GLUE methodology for Bayesian inversion that alleviates the problems associated with computationally costly models. Concepts from multilevel Monte Carlo and multilevel Markov-chain Monte Carlo methods are incorporated in the Generalized Likelihood Uncertainty Estimation (GLUE) methodology, resulting in the novel multilevel GLUE (MLGLUE) algorithm. In MLGLUE, a hierarchy of models with multiple resolutions (e.g., cell- or time-step sizes) are considered instead of using a (data-driven) surrogate model that is decoupled from the high-fidelity or target model. While surrogate models have been frequently used in place of computationally costly models to reduce the computational cost of statistical inversion, in MLGLUE the models on different levels in the hierarchy are synergetically used together and inferences using MLGLUE are made with respect to the target model instead of a surrogate. The evaluation of a parameter sample is initiated on the lowest level $\ell = 0$, which is associated with a computationally cheap low-resolution model. The sample is only passed to the next higher level $\ell+1$, which is associated with a model of higher resolution, if it results in a likelihood that is above a user defined threshold. Parameter samples are only finally accepted if they reach the highest level $\ell = L$, which is associated with the highest-resolution target model. Most parameter samples are evaluated (and discarded)

on lower levels and samples that reach the highest level are accepted with high probability, which results in substantial computational savings.

MLGLUE is evaluated using two test cases. The results of statistical inversion with MLGLUE are compared to the results from GLUE, Markov-chain Monte Carlo (MCMC) using a sampler from the DREAM family, as well as multilevel delayed acceptance (MLDA) MCMC in combination with a base-sampler from the DREAM family. There, identical numbers of prior samples are considered for all methods to ensure comparability. We show that the results (parameter posteriors, uncertainty estimates, convergence behaviour) for MLGLUE and GLUE are highly similar or even identical for both test cases. While the identified parameter posteriors are different for both test problems between GLUE, MLGLUE, MCMC, and MLDA, the resulting uncertainty estimates are similar. For the computationally more costly example of groundwater flow, MLGLUE results in the largest number of effective samples per minute and has the smallest overall computation time, reducing the time for inversion by $\approx$ 45% and $\approx$ 57% compared to conventional formulations of GLUE and MCMC, respectively. We expect the computational benefit of using MLGLUE to increase as the computational cost of a single model call increases, which has been previously identified for multilevel Monte Carlo and multilevel inversion (Cliffe et al., 2011; Giles, 2015; Dodwell et al., 2019; Lykkegaard et al., 2023).

As we discussed for both test cases and as mentioned by Lykkegaard et al. (2023), coarse levels should be designed carefully; i.e., lower-level models should be well correlated to the next higher level. While this is reflected in diagnostic plots as shown for the two examples, low or even negative correlation between levels will lead to parameter samples being discarded on lower levels although they would be accepted on higher levels, resulting in a smaller number of effective samples and in a smaller acceptance probability. Besides the samples of parameters and model outputs on the highest level, MLGLUE can optionally return these and other data for each model run on any level. This data enables the (statistical) analysis of various aspects such as the impact of model resolution on various quantities of interest or the possibility for model simplification. Savage et al. (2016) analyze the importance of model resolution via sensitivity analysis; analyzing the worth of aforementioned data from MLGLUE is an opportunity for future research, both in the context of multilevel methods and general model development.

Our results demonstrate that:

- By considering a hierarchy of models with decreasing (spatial) resolution, MLGLUE can substantially reduce the computational cost of statistical inversion for complex spatially distributed (groundwater) hydrological models.
- MLGLUE is most effective for PDE-based models, such as they are often encountered in the hydrological sciences; notions of grid or time-step refinement and coarsening are well understood in such cases and MLGLUE may be directly applied.
- MLGLUE can also be applied to problems with a generalized notion of resolution, e.g., when using different subsets of observation data.

MLGLUE enables statistical Bayesian inversion for models where it would previously have been computationally intractable, paving the way for more robust simulations and predictions of complex environmental systems under uncertainty.

Open Research Section

Relevant resources needed to reproduce the results as well as figures are openly available and can be found under the DOI `10.5281/zenodo.10018088` (Rudolph et al., 2023). The MLGLUE algorithm is available as a Python package under `https://github.com/iGW-TU-Dresden/MLGLUE`.

Acknowledgments

Funding for Thorsten Wagener has been provided by the Alexander von Humboldt Foundation in the framework of the Alexander von Humboldt Professorship endowed by the German Federal Ministry of Education and Research. The authors thank Robert Scheichl, Aretha Teckentrup, and Anastasia Istratuca for fruitful discussions and inspiration. The authors have no conflict of interest with respect to the results of this study.

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