Supporting Information for "Extending GLUE with Multilevel Methods to Accelerate Statistical Inversion of Hydrological Models"

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Introduction

This supporting information provides additional text and figures describing the results shown and discussed in the main article "Extending GLUE with Multilevel Methods to Accelerate Statistical Inversion of Hydrological Models". Texts S1 and S2 provide additional details on the derivation of MLGLUE. Texts S3 and S4 provide detailed descriptions of results and convergence behaviour for the example applicaitons of linear regression and groundwater flow, respectively. Figures S1 to S3 illustrate results for the linear regression example. Figures S4 to S6 illustrate results for the groundwater flow example.

Text S1 - Derivation of MLGLUE, the Wrong Combination of MLMC and GLUE

Assuming that likelihood thresholds are given on each level prior to sampling, a straightforward approach to combining MLMC and GLUE would be to use an MLMC algorithm (e.g., Giles, 2015) directly. Then, only model simulations would be considered that correspond to likelihoods that are above the level-dependent likelihood threshold. With that, as most MLMC samples come from lower levels, posterior parameter samples would mainly be comprised of samples from the posterior distribution corresponding to the coarser-level models. We aim, however, at generating samples that come from the posterior distribution on the finest level. This combination is therefore not purposeful. Otherwise we could directly use the model on level $\ell = 0$ to perform statistical inversion on a single level, which contradicts the actual aim of the methodology.

Text S2 - Derivation of MLGLUE, Level-Dependent Likelihood Thresholds

Using level-dependent likelihood thresholds instead of the highest-level threshold for all levels is motivated by the construction of the MLDA algorithm (Lykkegaard et al., 2023) as well as by the original delayed acceptance MCMC algorithm (Christen & Fox, 2005). In MLDA, different target densities are considered on each level because the likelihood function - seen as a (hyper-) surface in the parameter space - depends on the model used on a corresponding level. In the sense of Bayes' theorem, those densities can be considered to be Bayesian posterior densities. This is an intuitive construction; consider model evaluations on different levels, made with the same parameter samples, $\{\mathcal{F}_\ell(\boldsymbol{\theta}^{(i)}), \mathcal{F}_{\ell+1}(\boldsymbol{\theta}^{(i)})\}_{i=1}^N$, as well as corresponding likelihods $\{\widetilde{\mathcal{L}}_\ell(\boldsymbol{\theta}^{(i)}|\widetilde{\mathbf{Y}}), \widetilde{\mathcal{L}}_{\ell+1}(\boldsymbol{\theta}^{(i)}|\widetilde{\mathbf{Y}})\}_{i=1}^N$:

$$\mathcal{F}_\ell(\boldsymbol{\theta}_i) \neq \mathcal{F}_{\ell+1}(\boldsymbol{\theta}_i) \tag{1}$$

$$\Rightarrow \widetilde{\mathcal{L}}_\ell(\boldsymbol{\theta}^{(j)}|\widetilde{\mathbf{Y}}) \neq \widetilde{\mathcal{L}}_{\ell+1}(\boldsymbol{\theta}^{(j)}|\widetilde{\mathbf{Y}}) \tag{2}$$

$$\Rightarrow \widetilde{\mathcal{L}}_{T,\ell} \neq \widetilde{\mathcal{L}}_{T,\ell+1} \tag{3}$$

Therefore, level-dependent likelihood thresholds instead of a single highest-level threshold used on all levels need to be considered to accurately reflect the variations within the hierarchy of models.

Text S3 - Additional Description of Results, Linear Regression

The relations between levels for the case using a formally defined likelihood are shown in Fig. S1. For all different methods of inference results of the convergence analysis are shown in Fig. S2, parameter posterior distributions are shown in Fig. S3 (a) and (b), and uncertainty estimates are shown in Fig. S3 (c).

Neither $\mathbb{V}[\mathcal{F}_\ell]$ nor $\mathbb{E}[\mathcal{F}_\ell]$ are constant and neither $\mathbb{V}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ nor $\mathbb{E}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ decay as $\ell \to L$ for the case of using a formal likelihood (see Fig. S1); the approximation error therefore increases. Because the same exact samples are used for the analysis compared to using an informally defined likelihood function, it is apparent that individual parameter samples result in different likelihoods on different levels. This discrepancy can therefore be attributed fully to the differences in the likelihood functions (Eqs. 3 and 6 in the main article). Furthermore, using an informal likelihood results in substantially smaller variances and mean values on the different levels. While this suggests less sensitivity of the informal likelihood function to changes in model error, this corresponds to the aggregation of different sources of error and uncertainty in the likelihood function. Because this effect is superimposed by the effect of the likelihood functions having different codomains, it is not analyzed in more detail. Despite those discrepancies between the cases using formally or informally defined likelihood functions, posterior samples and uncertainty estimates are identical. This may be attributed to the fact that when a sample is passed to the next higher level $\ell + 1$ in the MLGLUE algorithm, only the likelihood on level ℓ serves as a decision threshold; likelihoods on levels $\ell - 1$ and $\ell + 1$ are not used for this decision. Because the ultimate decision on weather a parameter sample is considered behavioural is made on a single level (i.e., $\ell = L - 1$), the discrepancies between (average) likelihoods

on lower levels do not affect this decision. If, however, the likelihood threshold would be set to be equal to the highest-level threshold for all levels, many samples would be discarded on lower levels (as they are below the level-dependent threshold when $\mathbb{E}[\mathcal{F}_\ell]$ and $\mathbb{E}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ increase as $\ell \to L$), resulting in a strong effect on the final results.

With MLDA, a total number of $N_{\ell=L} = 400$ samples were computed on the highest level using $n_{chains} = 5$, resulting in a total of $N_{MLDA} = 400 * 5^2 * 5 = 100,000$ samples from the prior distribution. The first 50 samples were burnt from the 5 MLDA chains, resulting in $\widehat{R} = 1.02$ for both parameters. Out of the $3,755$ remaining samples, only 321 effective samples could be used (mean effective sample size estimate for the bulk of the posterior). Therefore, a thinning of 13 was applied, resulting in 289 effective samples. The first 500 samples are burnt from the 5 MCMC chains, resulting in $\widehat{R} = 1.00$ for both parameters. Out of the $97,505$ remaining samples, only $5,187$ effective samples could be used (mean effective sample size estimate for the bulk of the posterior). Therefore, a thinning of 19 was applied, resulting in $5,132$ effective samples.

More detailed results of the convergence analysis (see section 2.4 and Eq. 7 in the main article) are shown in Fig. S2. For each of the two parameters, MLGLUE and GLUE converge similarly; even for sample sizes as small as 4 the relative deviation from the global mean is within ±3%. MLDA requires a larger sample size of 20 for both parameters for $\mathcal{D}_{i,j}$ to continuously stay within ±3%. MCMC initially converges similarly to MLGLUE and GLUE, although a sample size of 40 is required for $\mathcal{D}_{i,j}$ to continuously stay within ±3%. The distributions of the bootstrap replicates of the normalized global mean are similar for MLGLUE, GLUE, and MLDA for both parameters; due to the large absolute

sample size, the correpsonding distribution of MCMC samples has a substantially smaller variance.

Text S4 - Additional Description of Results, Groundwater Flow

The relations between levels for the case using a formally defined likelihood are shown in Fig. S4. For all different methods of inference results of the convergence analysis are shown in Fig. S5, parameter posterior distributions are shown in Fig. S6 (a) - (d), and uncertainty estimates are shown in Fig. S6 (e) and (f).

When using the formal likelihood function (see Eq. 3 in the main article), $\mathbb{E}[\mathcal{F}_\ell]$ is approximately constant, while $\mathbb{V}[\mathcal{F}_\ell]$ increases as $\ell \to L$. $\mathbb{E}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$ decays as $\ell \to L$, showing that the approximation error decreases in mean; $\mathbb{V}[\mathcal{F}_\ell - \mathcal{F}_{\ell-1}]$, however, does not decay continuously and shows a particularly high value between levels $\ell = 2$ and $\ell = 1$ (see Fig. S4). As for the regression example, because the same exact samples are used for the analysis, the discrepancy between using a formal or informal likelihood can be attributed fully to the differences in the likelihood functions (Eqs. 3 and 6 in the main article). The magnitude of variance and mean are smaller for the case using an informal likelihood, suggesting that this formulation is less sensitive to changes in model error when different samples are evaluated. This may correspond to the aggregation of all sources of uncertainty and error in the informal likelihood function. However, that effect is mixed with the generally different codomains of the likelihood functions and is therefore not analyzed in more detail. Despite those discrepancies between the cases using formally or informally defined likelihood functions, estimated posteriors and uncertainty estimates are highly similar. The similarity may be attributed to the same model structure as the reference model being used and having independent Gaussian observation errors. Therefore, structural uncertainties are not projected onto parameters, as it is typically observed in practical applications of GLUE. However, this example demonstrates the

strong (conceptual) similarity between informal and formal definitions of the likelihood if assumptions regarding formality are actually met. The reader is referred to Vrugt, ter Braak, Gupta, and Robinson (2009) for a more detailled discussion regarding the effect of formal and informal Bayesian inference on uncertainty estimates in hydrological modelling.

With MLDA, a total number of $N_{\ell=L} = 16$ samples were computed on the highest level using $n_{chains} = 50$, resulting in a total of $N_{MLDA} = 16 * 5^3 * 50 = 100,000$ samples from the prior distribution. Only the initial sample was burnt from the 50 MLDA chains, resulting in a mean Gelman-Rubin statistic of $\overline{\widehat{R}} = 1.17$ ($\widehat{R}_{min} = 1.11$, $\widehat{R}_{max} = 1.26$), averaged over all 51 parameters. Out of the 800 remaining samples, only 311 effective samples could be used (mean effective sample size estimate for the bulk of the posterior). Therefore, a thinning of 3 was applied, resulting in 267 effective samples. Only the initial sample was burnt from the 50 MCMC chains, resulting in a mean Gelman-Rubin statistic of $\overline{\widehat{R}} = 1.10$ ($\widehat{R}_{min} = 1.07$, $\widehat{R}_{max} = 1.15$), averaged over all 51 parameters. Out of the $100,000$ remaining samples, only 386 effective samples can be used (mean effective sample size estimate for the bulk of the posterior). Therefore, a thinning of 260 was applied, resulting in 385 effective samples.

More detailed results of convergence analysis (see section 2.4 and Eq. 7 in the main article) are shown in Fig. S5. In a relative sense, GLUE shows the most rapid convergence for the PP parameters, followed by MCMC, MLGLUE, and MLDA. While MLGLUE, GLUE, and MLDA converge similarly for the length scale parameter, MCMC converges more rapidly. As for the regression example, MLGLUE, GLUE, and MLDA show similar distributions of the bootstrapped posterior mean, where the length scale parameter has

substantially smaller variance. The corresponding MCMC distributions have generally smaller variance compared to the other methods. Taking the comparable numbers of effective posterior samples into account and while all methods converge similarly, multilevel methods are more efficient in that the overall computational cost is substantially lower compared to single-level methods.

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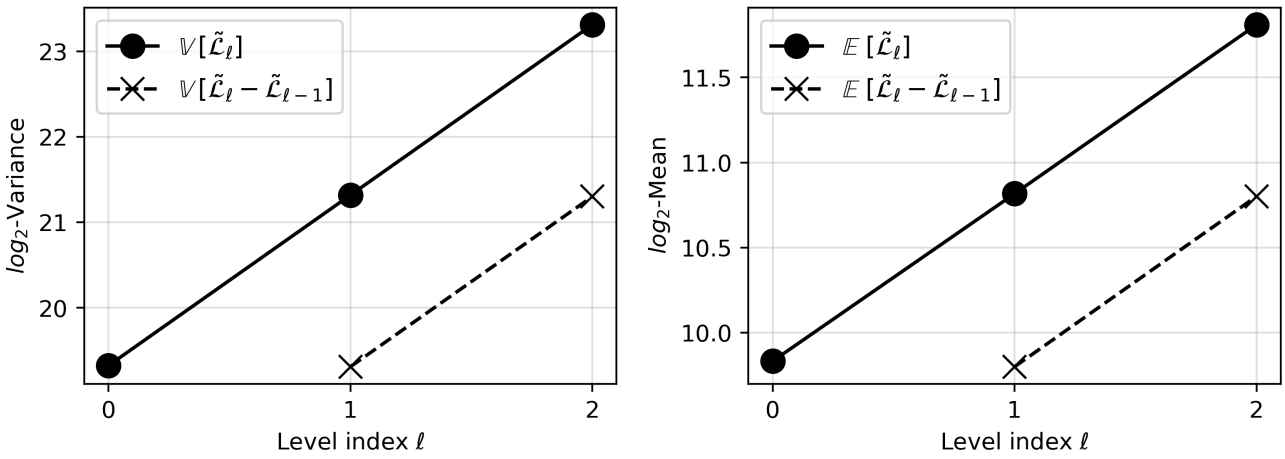

Figure S1. Relations between levels for the linear regression example, using a formal definition of the likelihood

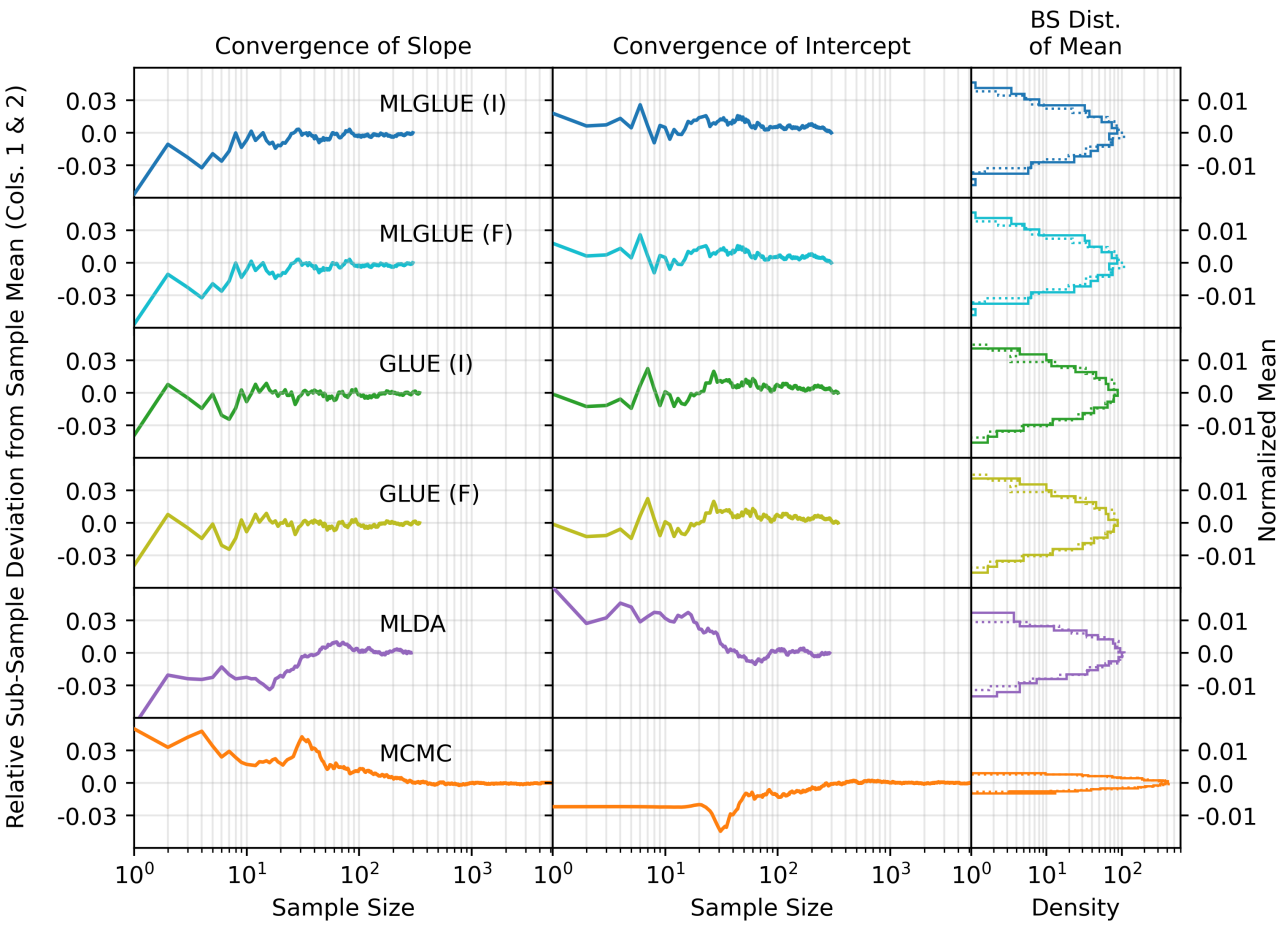

Figure S2. Convergence analysis for the linear regression example; the rightmost column shows the distribution of normalized bootstrap replicates of the posterior mean (solid line for slope, dotted line for intercept); (F) stands for a formal likelihood and (I) stands for an informal likelihood

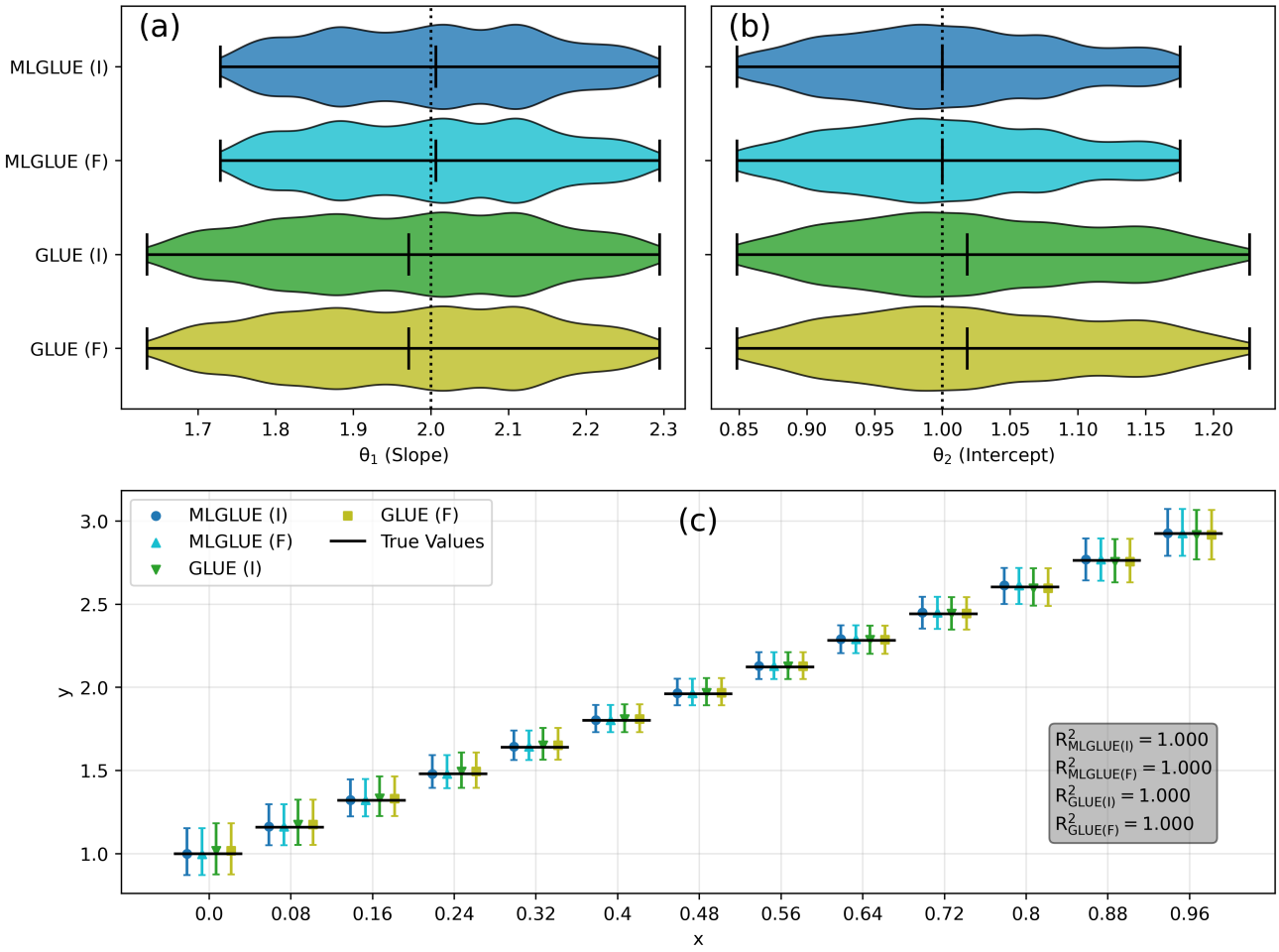

Figure S3. Kernel density estimates of model parameters, where solid vertical lines represent distribution median values and dashed lines represent the true parameter values (a, b) and $99\% - 1\%$ uncertainty estimates around the median value (c); (F) stands for a formal likelihood and (I) stands for an informal likelihood

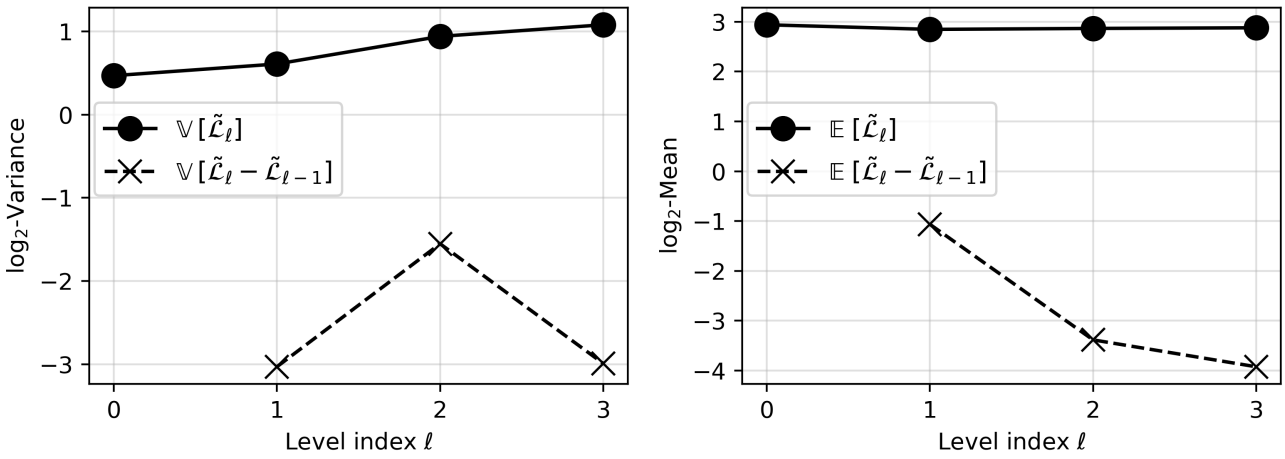

Figure S4. Relations between levels for the groundwater flow example, using a formal definition of the likelihood

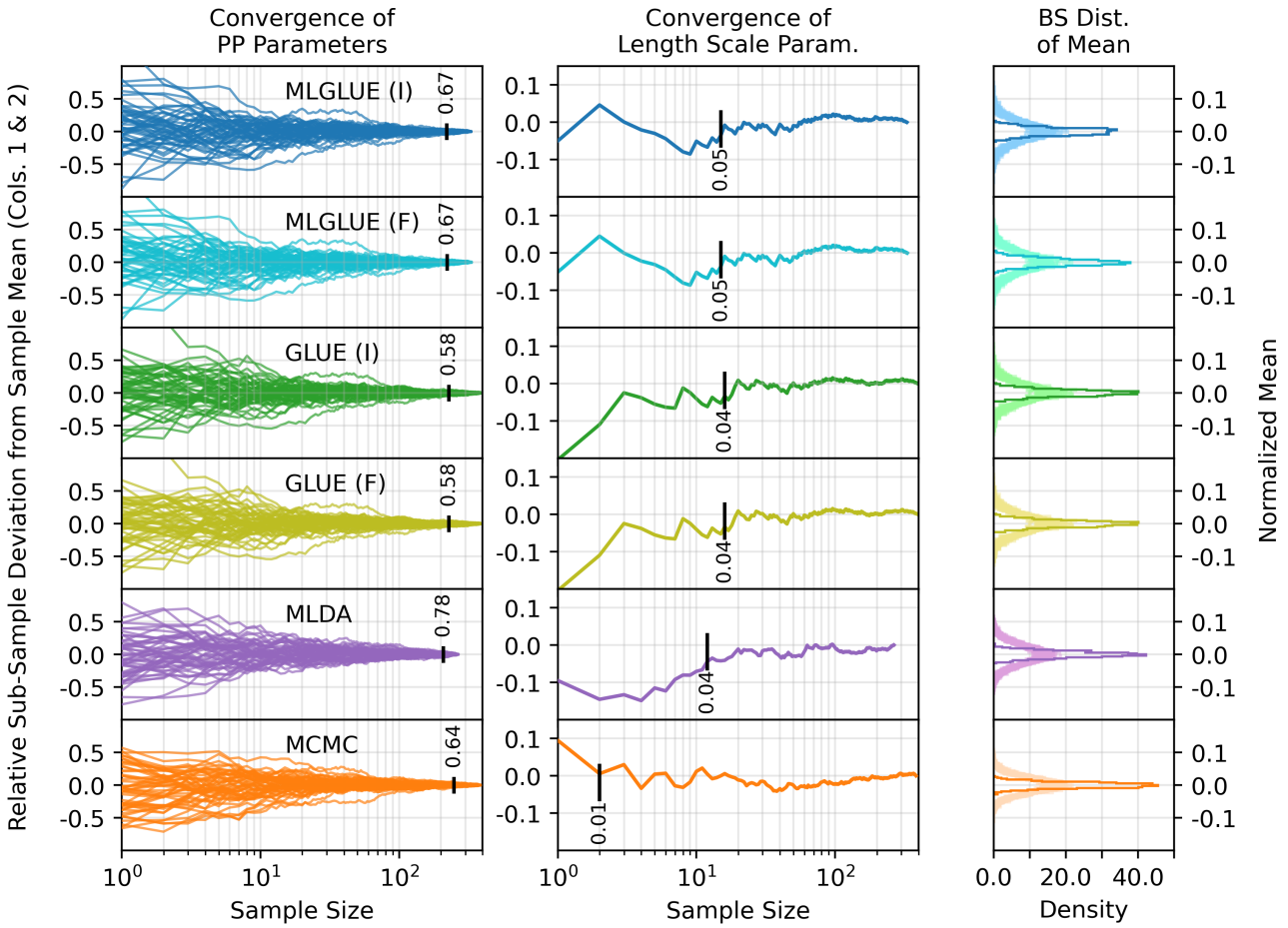

Figure S5. Convergence analysis for the groundwater flow example; the rightmost column shows the distribution of normalized bootstrap replicates of the posterior mean (lighter lines for PP parameters, darker line for GPR length scale); vertical lines represent the fraction of the global sample sizes at which $D_{i,j}$ continuously stays within 5%; (F) stands for a formal likelihood and (I) stands for an informal likelihood

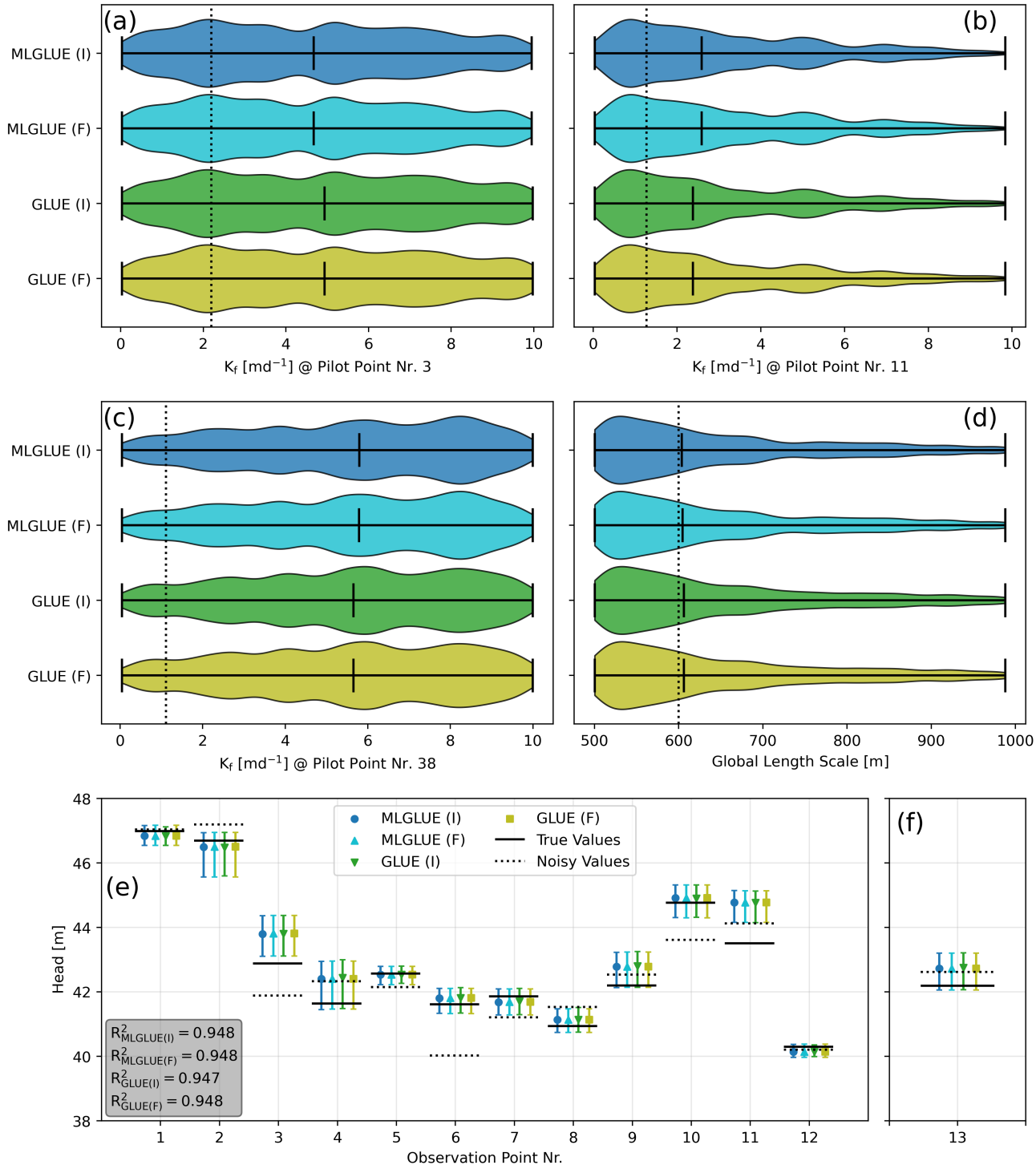

Figure S6. Kernel density estimates of model parameters, where solid vertical lines represent distribution median values and dashed lines represent the true parameter values (a, b, c, d) and $99\% - 1\%$ uncertainty estimates around the median value for observation points (e) and for the prediction point(f); (F) stands for a formal likelihood and (I) stands for an informal likelihood