Component-wise iterative ensemble Kalman inversion for static Bayesian models with unknown measurement error covariance

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Abstract

The ensemble Kalman filter (EnKF) is a Monte Carlo approximation of the Kalman filter for high dimensional linear Gaussian state space models. EnKF methods have also been developed for parameter inference of static Bayesian models with a Gaussian likelihood, in a way that is analogous to likelihood tempering sequential Monte Carlo (SMC). These methods are commonly referred to as ensemble Kalman inversion (EKI). Unlike SMC, the inference from EKI is asymptotically biased if the likelihood is non-linear and/or non-Gaussian and if the priors are non-Gaussian. However, it is significantly faster to run. Currently, a large limitation of EKI methods is that the covariance of the measurement error is assumed to be fully known. We develop a new method, which

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we call component-wise iterative EKI (CW-IEKI), that allows elements of the covariance matrix to be inferred alongside the model parameters at negligible extra cost. This novel method is compared to SMC on a linear Gaussian example as well as four examples with non-linear dynamics (i.e. non-linear function of the model parameters). The non-linear examples include a set of population models applied to synthetic data, a model of nitrogen mineralisation in soil that is based on the Agricultural Production Systems Simulator, a model predicting seagrass decline due to stress from water temperature and light, and a model predicting coral calcification rates. On our examples, we find that CW-IEKI has relatively similar predictive performance to SMC, albeit with greater uncertainty, and it has a significantly faster run time.

**Keywords:** Bayesian inference, EKI, SMC, APSIM, seagrass, coral, model sloppiness

(Some figures may appear in colour only in the online journal)

1. Introduction

1.1. Problem description

Consider the following statistical model

\[ y = G(\theta) + \eta, \quad \eta \sim \mathcal{N}(0, \Gamma(\phi)) \]

where \( y \in Y \subseteq \mathbb{R}^{d_y \times 1} \) are the observations, \( \theta \in \Theta \subseteq \mathbb{R}^{d_\theta \times 1} \) and \( \phi \in \Phi \subseteq \mathbb{R}^{d_\phi \times 1} \) are the parameters, \( G : \Theta \rightarrow Y \) is a deterministic mathematical model, and \( \eta \in Y \) are the measurement errors. We use \( \mathcal{N}(y | \mu, \Sigma) \) to denote the multivariate normal or Gaussian distribution evaluated at \( y \) and with mean vector \( \mu \) and covariance \( \Sigma \). The number of observations is \( d_y \), the number of parameters is \( d_\theta + d_\phi \) and \( \Gamma(\phi) \in \mathbb{R}^{d_y \times d_y} \) is the covariance matrix characterising the measurement errors. Our interest is in the posterior distribution of \((\theta, \phi)\) conditional on the observed data \( y \),

\[ \pi(\theta, \phi | y) \propto \mathcal{N}(y | G(\theta), \Gamma(\phi))p(\theta, \phi), \]

where \( \mathcal{N}(y | G(\theta), \Gamma(\phi)) \) is the Gaussian likelihood function and \( p(\theta, \phi) \) is the prior density of \( \theta \) and \( \phi \). For ease of notation, we omit the dependence on the fixed \( y \) in the rest of the paper. Additionally, we use \( \pi(\cdot) \) as shorthand for \( \pi(\theta | \phi, y) \propto \mathcal{N}(y | G(\theta), \Gamma(\phi))p(\theta) \), where \( y \) and \( \phi \) are assumed to be known and fixed.

Markov chain Monte Carlo (MCMC; Robert and Casella 1999) or sequential Monte Carlo (SMC; Del Moral et al 2006) methods can be used for asymptotically exact parameter inference of \( \theta \) and \( \phi \). These methods generally require many evaluations of \( G(\cdot) \), however, which limits their feasibility when \( G(\cdot) \) is computationally expensive to evaluate.

If the elements of \( \phi \) are known, methods based on the ensemble Kalman filter (EnKF; Evensen 1994, Burgers et al 1998, Le Gland et al 2009, Roth et al 2017) are a fast but inexact alternative to MCMC and SMC. EnKF for inverse problems is generally known as ensemble Kalman inversion (EKI; Iglesias et al 2013). In the Bayesian setting, EKI methods simulate an initial ensemble from the prior, and iteratively updates it to capture statistical properties of the EKI approximation \( \hat{\pi}(\theta) \) to the posterior \( \pi(\theta) \). If the EKI algorithm is iterated long enough, i.e. as the number of iterations \( J \) approaches infinity, the ensemble will collapse to a single
point minimising the loss function $||y - G(\theta)||_{\Gamma}$. For uncertainty quantification, i.e. to sample from $\tilde{\pi}(\theta)$, early stopping of the algorithm is essential (Iglesias et al 2013). In general, EKI is only exact in the linear setting. If $G(\cdot)$ is a linear function and the prior is Gaussian, then, as the number of samples ($N$) approaches infinity, a single iteration of EKI provides exact samples from the posterior (Iglesias 2014, Duffield and Singh 2022), and the mean of the ensemble converges to the maximum \textit{a posteriori} estimate (Iglesias et al 2013).

Currently, EKI methods require the covariance $\Gamma$ to be fully specified. We aim to extend EKI for estimation and uncertainty quantification of models where $\Gamma$ has unknown elements $\phi$, i.e. we give an extension that samples from an approximation to $\pi(\theta, \phi | y)$ instead of an approximation to $\pi(\theta | \phi, y)$.

1.2. Previous EKI approaches

EKI methods were originally developed for derivative-free optimisation (Li and Reynolds 2009, Iglesias et al 2013), and later extended to sample from the posterior distribution (Garbuno-Inigo et al 2020, Ding and Li 2021, Huang et al 2021, Reich and Weissmann 2021). Convergence results for EKI as an optimiser is developed in the continuous time limit (for a fixed ensemble size) for linear (Schillings and Stuart 2017a, 2017b, Blömker et al 2018, 2019, 2021) and non-linear (Blömker et al 2021) models. Theoretical properties of EKI as a sampler is investigated by Garbuno-Inigo et al (2020), Ding and Li (2021) and Huang et al (2022) in the continuous time limit and by Ernst et al (2015) as the number of iterations and the ensemble size approach infinity.

As inverse problems are often ill-posed, an active area of research is how to incorporate regularisation in EKI. By construction, EKI is regularised through the subspace property, i.e. that the final ensemble is in the linear span of the initial ensemble (Li and Reynolds 2009, Iglesias et al 2013). Additional regularisation may be necessary to improve its robustness and stability however (Iglesias et al 2013). EKI methods incorporating Tikhonov regularisation (TEKI) are developed and studied by Iglesias (2016), Chada et al (2020), Chada and Tong (2021) and Lee (2021), with adaptive schemes given by Iglesias and Yang (2021), Weissmann et al (2022) and Parzer and Scherzer (2022). An alternative to TEKI is the tempering approach of Iglesias (2014), which scales the covariance of the noise ($\Gamma$) by some stepsize $\alpha$. Adaptation strategies for $\alpha$ are given by Iglesias et al (2018) and Iglesias and Yang (2021), and correspond to a type of covariance inflation.

We focus on EKI as a posterior sampler. For linear models, EKI samples from the exact posterior distribution, but its performance for general models is not well understood. For EKI with a fixed stepsize ($\alpha = 1$), Ernst et al (2015) show that the covariance of the final ensemble does not approximate the posterior covariance for non-linear models as it is independent of the observed data $y$. Recent variants of EKI aim to improve its performance as a sampler. The ensemble Kalman sampler of Garbuno-Inigo et al (2020) (see also Ding and Li 2021) perturbs the ensemble instead of the observations as in regular EKI, Duffield and Singh (2022) extend EKI for non-Gaussian likelihoods through a Gaussian approximation of the likelihood, Rammay et al (2020) explicitly incorporates error arising from model misspecification, and Iglesias et al (2018) relates the tempering method of Iglesias (2014) to likelihood tempering SMC and uses ideas from SMC to adaptively select the stepsize at each iteration. Since the likelihood is Gaussian, the latter approach targets an approximation to the power posterior at iteration $j$

$$\tilde{\pi}_j(\theta) \approx \pi_j(\theta) \propto N(y | G(\theta), \alpha_j \Gamma)p(\theta) \propto N(y | G(\theta), \Gamma)p(\theta)$$

$$\approx \pi(\theta, \phi | y)$$
where \(0 \leq \alpha_j \leq 1\) is the regularisation parameter at iteration \(j\) and \(\alpha_{j+1} > \alpha_j\) for \(j = 0, \ldots, J - 1\) (Iglesias et al 2018). We refer to the approach of Iglesias et al (2018) as iterative EKI (IEKI).

Currently, a limiting factor of these methods is that the covariance of the noise \(\Gamma(\phi)\) is assumed to be known. A partial exception is the method of Rammay et al (2020), which incorporates error from model misspecification using a fraction of the data residual at each iteration, i.e. the difference between the observed data and the model outputs. The covariance matrix \(\Gamma\) is still assumed to be known and fixed, but it is adaptively inflated with the extra error term. A comparison of the method of Rammay et al (2020) and density tempering SMC is provided in Vilas et al (2021).

1.3. Our contribution

In this paper we develop a new adaptive EKI method, which we call component-wise IEKI (CW-IEKI), that can handle the common situation where the noise parameters \(\phi\) are unknown and require estimation. This new method extends that of Iglesias et al (2018) by sampling from the EKI approximation to the posterior distribution of \(\theta | \phi, y\), then sampling from the exact posterior distribution of \(\theta | \theta, y\). Our method is completely analogous to density tempering SMC, which permits a direct comparison with the latter in terms of posterior accuracy and computation time. In this paper we illustrate the new CW-IEKI method and perform comparisons on a linear Gaussian model, a set of population models and three other real models: a model of nitrogen mineralisation in soil that is based on the Agricultural Production Systems Simulator (APSIM) with partially known noise (Vilas et al 2021), a model predicting seagrass decline due to cumulative stress from water temperature and light (Adams et al 2020), and a model for predicting coral calcification rates (Galli and Solidoro 2018).

The rest of the paper is organised as follows. Section 2 gives the background on EnKF, particle filters, likelihood tempering SMC, and EKI methods. Section 3 describes our novel CW-IEKI method and section 4 compares the performance of our method on a linear Gaussian model and four ecological model examples. Section 5 concludes with a discussion of potential future work.

2. Background

This section describes the filtering problem and the solutions given by the EnKF (Evensen 1994) and the bootstrap particle filter (Gordon et al 1993). It also describes how likelihood tempering SMC and EKI can be used for parameter inference of the static model given in equation (1). We use the notation \(z_{ij} := \{z_i, z_{i+1}, \ldots, z_j\}^T\) for \(j \geq i\) throughout. We also use \(p\) as general notation for a probability density throughout the paper.

2.1. EnKF

The Kalman filter and the EnKF were developed to solve the filtering problem for state space models (SSMs)—this is often referred to as state estimation or data assimilation. Consider an SSM of the form

\[
Y_t \mid (X_t = x_t) \sim g(y_t \mid x_t), \\
X_t \mid (X_{t-1} = x_{t-1}) \sim f(x_t \mid x_{t-1}), \\
X_0 \sim \mu(x_0),
\]

(2)
where \( y_{1:T} \) are the observed data, \( x_{0:T} \) are the unobserved or latent states and \( T \) is the number of observations. The filtering distribution, \( p(x_t \mid y_{1:t}) \), can be solved by recursively applying the time update

\[
p(x_t \mid y_{1:t-1}) = \int f(x_t \mid x_{t-1})p(x_{t-1} \mid y_{1:t-1}) \, dx_{t-1}.
\]

and the measurement update

\[
p(x_t \mid y_{1:t}) = \frac{g(y_t \mid x_t)p(x_t \mid y_{1:t-1})}{p(y_t \mid y_{1:t-1})}.
\]

Note that \( p(x_0 \mid y_{1:0}) = \mu(x_0) \) is assumed to be known. See chapter 3 of Schön and Lindsten (2017) for more detail on the filtering problem and its solution. The Kalman filter solves (3) and (4) analytically for linear Gaussian SSMs (LG-SSMs),

\[
Y_t \mid (X_t = x_t) \sim \mathcal{N}(y_t \mid Hx_t, R),
\]

\[
X_t \mid (X_{t-1} = x_{t-1}) \sim \mathcal{N}(x_t \mid Fx_{t-1}, Q),
\]

\[
X_0 \sim \mathcal{N}(x_0 \mid \bar{x}_0, C_0^a),
\]

where \( y_t \subseteq \mathbb{R}^{d_y \times 1} \) and \( x_t \subseteq \mathbb{R}^{d_x \times 1} \). The quantities \( H \subseteq \mathbb{R}^{d_y \times d_x} \), \( R \subseteq \mathbb{R}^{d_y \times d_y} \), \( \bar{x}_0 \subseteq \mathbb{R}^{d_x \times 1} \) and \( F, Q, C_0^a \subseteq \mathbb{R}^{d_x \times d_x} \) are assumed to be known. Here, the time (3) and measurement (4) updates are

\[
p(x_t \mid y_{1:t-1}) = \mathcal{N}(x_t \mid \bar{x}_t, C_t^a),
\]

\[
\bar{x}_t = F\bar{x}_{t-1},
\]

\[
C_t^a = FC_{t-1}^aF^T + Q,
\]

and

\[
p(x_t \mid y_{1:t}) = \mathcal{N}(x_t \mid \tilde{x}_t, C_t^a),
\]

\[
\tilde{x}_t = \bar{x}_t + K_t(y_t - \hat{y}_t),
\]

\[
C_t^a = (I - K_tH)C_t^a,
\]

respectively, where \( \hat{y}_t = H\bar{x}_t \) and \( I \in \mathbb{R}^{d_x \times d_x} \) is the identity matrix. The Kalman gain at time \( t \) is

\[
K_t = C_t^{\tilde{x}y} \left( C_t^{\tilde{x}\tilde{x}} \right)^{-1} = C_t^{\tilde{x}y}H^T \left( HC_t^{\tilde{x}y}H^T + R \right)^{-1},
\]

where \( C_t^{\tilde{x}y} \) is the cross covariance between \( \tilde{x}_t \) and \( \hat{y}_t \), \( C_t^{\tilde{x}\tilde{x}} \) is the covariance of \( \tilde{x}_t \), and \( C_t^{\tilde{x}y} \) is the covariance of \( \tilde{x}_t \).

The EnKF is a Monte Carlo approximation of the Kalman filter for LG-SSMs. For nonlinear, non-Gaussian SSMs, EnKF is asymptotically biased. The EnKF simulates the initial ensemble from the prior \( x_0^n \sim \mu(x_0) \) for \( n = 1, \ldots, N \), then updates the ensemble for each iteration as follows. First, the state and observation predictions are simulated

\[
\tilde{x}_t^n \sim f(\cdot \mid \tilde{x}_{t-1}^n),
\]

\[
\hat{y}_t^n \sim g(\cdot \mid \tilde{x}_t^n),
\]
for \( n = 1, \ldots, N \). In the linear case, \( \tilde{x}_{i-1}^n \sim p(x_{t-1} \mid y_{1:t-1}) \), and \( \tilde{x}_{i}^n \sim p(x_{t} \mid y_{1:t-1}) \). Then, the ensemble is given by

\[
\tilde{x}_{i}^n = \tilde{x}_{i}^n + \hat{C}_t^{\tilde{\gamma}} \left( \hat{C}_t^{\tilde{\gamma}} \right)^{-1} (\tilde{y}_i - \tilde{y}_i) ,
\]

where \( \hat{C}_t^{\tilde{\gamma}} \) is the sample cross covariance between \( \tilde{x}_i \in \mathbb{R}^{d_t \times N} \) and \( \tilde{y}_i \in \mathbb{R}^{d_y \times N} \),

\[
\hat{C}_t^{\tilde{\gamma}} = \frac{1}{N-1} \sum_{n=1}^{N} \left( \tilde{x}_i^n - \frac{1}{N} \sum_{j=1}^{N} \tilde{x}_i^j \right) \left( \tilde{y}_i^n - \frac{1}{N} \sum_{j=1}^{N} \tilde{y}_i^j \right)^\top ,
\]

and \( \hat{C}_t^{G} \) is the sample covariance of \( \tilde{y}_i \in \mathbb{R}^{d_y \times N} \)

\[
\hat{C}_t^{G} = \frac{1}{N-1} \sum_{n=1}^{N} \left( \tilde{y}_i^n - \frac{1}{N} \sum_{j=1}^{N} \tilde{y}_i^j \right) \left( \tilde{y}_i^n - \frac{1}{N} \sum_{j=1}^{N} \tilde{y}_i^j \right)^\top .
\]

For LG-SSMs, \( \tilde{x}_{i}^n \sim p(x_{t} \mid y_{1:t}) \). Note that we follow Iglesias et al. (2018) and use a factor of \( 1/(N-1) \) to calculate the sample covariances throughout the paper instead of \( 1/N \). This ensures that the estimated covariances are unbiased even when the ensemble size \( N \) is small. Further, when \( N \) is relatively large, e.g. \( N \geq 100 \), we do not expect to see any meaningful differences in the results. If the observation density is Gaussian, i.e. \( g(y_t \mid x_t) = \mathcal{N}(y_t \mid G(x_t), \Gamma) \) with known covariance \( \Gamma \), the Monte Carlo error in the calculation of the covariance matrices can be reduced (Roth et al. 2017). Let \( \tilde{g}_i^n = G(\tilde{x}_i^n) \), then the sample cross covariance and sample covariance defined in equations (5) and (6) become

\[
\hat{C}_t^{\tilde{\gamma}} = \frac{1}{N-1} \sum_{n=1}^{N} \left( \tilde{g}_i^n - \frac{1}{N} \sum_{j=1}^{N} \tilde{g}_i^j \right) \left( \tilde{x}_i^n - \frac{1}{N} \sum_{j=1}^{N} \tilde{x}_i^j \right)^\top ,
\]

\[
\hat{C}_t^{G} = \frac{1}{N-1} \sum_{n=1}^{N} \left( \tilde{g}_i^n - \frac{1}{N} \sum_{j=1}^{N} \tilde{g}_i^j \right) \left( \tilde{g}_i^n - \frac{1}{N} \sum_{j=1}^{N} \tilde{g}_i^j \right)^\top + \Gamma .
\]

2.2. Particle Filters

For non-linear, non-Gaussian SSMs, SMC methods give an exact solution to the filtering problem. SMC methods for dynamic models are often referred to as particle filters. As with EnKF, the bootstrap particle filter (Gordon et al. 1993) draws an initial ensemble from the prior \( \mu(x_0) \). The particle filter then transforms the prior ensemble to samples from the filtering distribution through a sequence of reweighting, resampling and mutation steps. Given a set of weighted samples, \( \{\tilde{x}_{n-1}^n, W_{n-1}^n\}_{n=1}^{N} \sim p(x_{t-1} \mid y_{1:t-1}) \), the bootstrap particle filter maps these to \( p(x_t \mid y_{1:t}) \) as follows:

1. Resample the particles according to their weights, \( W_{n-1}^n \), and set \( W_{n-1}^n = 1/N \) for \( n = 1, \ldots, N \). This gives a set of evenly weighted particles \( \{\tilde{x}_{n-1}^n, \frac{1}{N}\}_{n=1}^{N} \) distributed according to \( p(x_{t-1} \mid y_{1:t-1}) \).
2. Simulate the state predictions using the transition density \( \hat{p}(\cdot \mid \tilde{x}_{n-1}^n) \), which gives a set of unweighted particles distributed according to \( p(x_t \mid y_{1:t-1}) \).
Reweight the particles using the observation density \( w_n^o = g(y_t | \tilde{x}_n^o) \) for \( n = 1, \ldots, N \) and normalise the weights to get \( W_j^{1:N} \). The final set of weighted particles is distributed according to \( p(x_t | y_{1:t}) \).

Steps 1–3 are iterated until all \( T \) observations have been processed. When \( t = 0 \), \( p(x_0 | y_{1:0}) = \mu(x_0) \).

2.3. Likelihood tempering SMC

SMC can also be used to sample from the static model given in equation (1) (Del Moral et al 2006). SMC methods require a sequence of distributions, \( \pi_0(\theta, \phi), \ldots, \pi_J(\theta, \phi) \) to be defined, where \( \pi_j(\theta, \phi) \) is equal to the desired posterior distribution \( \pi(\theta, \phi) \). A common approach is likelihood tempering SMC, which raises the likelihood function to a power \( \alpha_j, j = 0, \ldots, J \), where \( \alpha_0 = 0 < \alpha_1 < \cdots < \alpha_J = 1 \). At iteration \( j \), the power posterior \( \pi_j(\theta, \phi) \propto p(y | \theta, \phi)^\alpha_j p(\theta, \phi) \) is targeted. Note that \( \pi_0(\theta, \phi) = p(\theta, \phi) \) is the prior and \( \pi_j(\theta, \phi) \propto p(y | \theta, \phi)p(\theta, \phi) \) is the posterior distribution.

Given a set of evenly weighted samples from \( \pi_{j-1}(\theta, \phi) \), likelihood tempering SMC transforms these to samples from \( \pi_j(\theta, \phi) \) as follows:

1. Reweight the particles using the ratio of the current target to the previous target, \( w_n^o = \pi_j(\theta_{j-1}, \phi_{j-1}) / \pi_{j-1}(\theta_{j-1}, \phi_{j-1}) \) for \( n = 1, \ldots, N \) and normalise the weights to get \( W_j^{1:N} \). This gives a set of weighted particles that are distributed according to \( \pi_j(\theta, \phi) \).
2. Resample the particles according to their weights, and set \( W_{j-1}^n = 1/N \) for \( n = 1, \ldots, N \).
3. Mutate the resampled particles using an MCMC kernel which targets the distribution \( \pi_j(\theta, \phi) \).

Step 2 removes the negligible weight particles and duplicates the high weight particles, and step 3 diversifies the particles to mitigate the duplication. A common approach to mutate the particles is to use \( M \) iterations of an MCMC algorithm with \( \pi_j(\theta, \phi) \) as its invariant distribution.

The tempering parameter \( \alpha_j \) can be adapted at each iteration by setting \( \alpha_j \) such that a pre-specified effective sample size (ESS) threshold is achieved (Jasra et al 2010). The algorithm stops once \( \alpha_j = \alpha_J = 1 \). This will be some proportion of \( N \). While the ESS cannot be calculated exactly, it can be approximated at each iteration \( j \) using the normalised weights \( W_j^{1:N} \),

\[
\text{ESS}_j = \frac{1}{\sum_{n=1}^{N} W_n^o}.
\]

Note that the unnormalised weights at iteration \( j \) is given by

\[
w_j = \frac{\pi_j(\theta_{j-1}, \phi_{j-1})}{\pi_{j-1}(\theta_{j-1}, \phi_{j-1})} = \frac{p(y | \theta_{j-1}, \phi_{j-1})^{\alpha_j} p(\theta_{j-1}, \phi_{j-1})}{p(y | \theta_{j-1}, \phi_{j-1})^{\alpha_{j-1}} p(\theta_{j-1}, \phi_{j-1})} = p(y | \theta_{j-1}, \phi_{j-1})^{\alpha_j - \alpha_{j-1}}.
\]

Since the parameter \( \alpha_j \) is adapted before the reweighting step, the weights can be written as a function of \( \alpha_j \). Thus, the ESS in (9) can also be written as a function of \( \alpha_j \), i.e. \( \text{ESS}_j(\alpha_j) \). At every iteration, \( \alpha_j \) is selected such that \( \alpha_{j-1} \leq \alpha_j \leq 1 \) and \( \text{ESS}_j(\alpha_j) \) is equal to the specified ESS threshold. Note that when \( \alpha_j = \alpha_J = 1 \), \( \text{ESS}_j(1) \) will be greater than or equal to the specified threshold.

If the function \( G(\cdot) \) in equation (1) is expensive to compute, SMC may be prohibitively expensive to run. Each iteration \( j = 1, \ldots, J \) requires a minimum of \( NM_j \) evaluations of \( G(\cdot) \),
where $M_j$ is the number of MCMC repeats in iteration $j$. The entire algorithm requires a minimum of $N \sum_{j=1}^{J} M_j + 1$ evaluations, where the extra evaluation comes from the initial calculation of the likelihood. A less expensive, but asymptotically biased alternative to SMC for static models is EKI.

### 2.4. EKI

Iglesias et al (2013) extend the EnKF algorithm for static models with known $\Gamma(\phi)$ by introducing artificial dynamics. Since $\Gamma(\phi)$ is assumed to be known, we omit the dependence on $\phi$. The static model in equation (1) can be constructed from the general SSM in equation (2) by setting the transition density to the identity function and denoting $x_t = \theta_j$, i.e. $f(x_t = x_{t-1}) = \theta_j$. The EnKF artificial time update is then $\tilde{\theta}_j^n = \theta_{j-1}^n$ for $n = 1, \ldots, N$ and the measurement update is $\theta_j^n = \tilde{\theta}_j^n + C_j^{\tilde{\phi}}(\tilde{C}_j^{\tilde{\phi}})^{-1}(x_j - \tilde{x}_j^n)$, where $\tilde{x}_j^n \sim \mathcal{N}(\cdot | G(\tilde{\theta}_j^n), \Gamma)$. The EKI algorithm of Iglesias et al (2013) for static Bayesian models proceeds as below:

1. Sample $\theta_0^n \sim p(\theta)$ for $n = 1, \ldots, N$.
2. Update $\theta_j^n = \tilde{\theta}_j^n + C_j^{\tilde{\phi}}(\tilde{C}_j^{\tilde{\phi}})^{-1}(y - \tilde{x}_j^n)$ where $\tilde{\theta}_j^n = \theta_{j-1}^n$ and $\tilde{x}_j^n \sim \mathcal{N}(G(\tilde{\theta}_j^n), \Gamma)$ for $n = 1, \ldots, N$.
3. Iterate step 2 as desired.

Since the likelihood $p(y \mid \theta)$ is Gaussian, equations (7) and (8) are used for the covariance calculations. In equation (7), the ensemble $\tilde{x}_k \in \mathbb{R}^{d_x \times N}$ is replaced with $\tilde{\theta}_j \in \mathbb{R}^{d_\theta \times N}$.

While the prior induces regularisation through the subspace property, additional regularisation is often required to properly explore regions of high posterior support without overfitting the data (Iglesias 2014). An iteratively regularised extension of the EKI method of Iglesias et al (2013) is the algorithm of Iglesias et al (2018):

1. Sample $\theta_0^n \sim p(\theta)$ for $n = 1, \ldots, N$.
2. Update $\theta_j^n = \tilde{\theta}_j^n + C_j^{\tilde{\phi}}(\tilde{C}_j^{\tilde{\phi}})^{-1}(y - \tilde{x}_j^n)$ where $\tilde{\theta}_j^n = \theta_{j-1}^n$ and $\tilde{x}_j^n \sim \mathcal{N}(G(\tilde{\theta}_j^n), (\alpha_j - \alpha_{j-1})^{-1}\Gamma)$ for $n = 1, \ldots, N$.
3. Iterate step 2 until $\alpha_j = \alpha_j = 1$.

Here, (8) becomes

$$C_j^{\tilde{\phi}} = \frac{1}{N - 1} \sum_{n=1}^{N} \left( \tilde{g}_j^n - \frac{1}{N} \sum_{k=1}^{N} \tilde{g}_j^k \right) \left( \tilde{g}_j^n - \frac{1}{N} \sum_{k=1}^{N} \tilde{g}_j^k \right)^\top + \frac{1}{\alpha_j - \alpha_{j-1}} \Gamma.$$

We refer to this method as IEKI. Similar to likelihood tempering SMC, IEKI also targets a sequence of distributions $\tilde{\pi}_0(\theta), \ldots, \tilde{\pi}_J(\theta)$. At iteration $j$, the algorithm targets $\tilde{\pi}_j(\theta)$, which approximates

$$\pi_j(\theta) \propto \mathcal{N}(y \mid G(\theta), \Gamma)^\alpha p(\theta).$$

Note that $\pi_j(\theta)$ is exactly the $j$th target in the likelihood tempering SMC algorithm defined in section 2.3.
The parameter $\alpha_j$ can be chosen adaptively for $j = 1, \ldots, J$ (Iglesias et al. 2018). At iteration $j$, assume that the particles must be reweighted from $\tilde{\pi}_{j-1}(\theta)$ to $\tilde{\pi}_j(\theta)$. Analogously to likelihood tempering SMC, these weights are given by

$$w_j^j = \pi_j \left( \frac{\theta_{j-1}^n}{\pi_{j-1} \left( \theta_{j-1}^n \right)} \right) \propto \exp \left(-\frac{\alpha_j - \alpha_{j-1}}{2} \left(y - G \left( \theta_{j-1}^n \right) ^\top \Gamma^{-1} \left(y - G \left( \theta_{j-1}^n \right) \right)\right) \right),$$

where the obtained $w_j^{1:N}$ are thereafter normalised to give $\tilde{W}_j^{1:N}$. The parameter $\alpha_j$ is set so that the ESS, estimated using (9), matches some target threshold. The function $G(\cdot)$ is evaluated once per particle at every iteration, so that the total number of evaluations for IEKI is $JN$, where $J$ is the total number of iterations and $N$ is the number of particles or the ensemble size. This is much less than the computation required for SMC, but IEKI assumes that $\Gamma$ is known. In the next section we develop a new adaptive EKI method that can estimate unknown parameters associated with $\Gamma$.

3. CW-IEKI

A strong limitation of EKI in general is that $\Gamma$ must be known. We extend IEKI to the case where $\Gamma$ depends on some unknown parameter or parameters $\phi$. For example, in the simplest case, this might be $\Gamma(\phi) = \phi I$, where $I \in \mathbb{R}^{d \times d}$ is the identity matrix, although our method does not require this assumption to hold. The target distribution at iteration $j$ is $\tilde{\pi}_j(\theta, \phi)$, which approximates

$$\pi_j(\theta, \phi) \propto \mathcal{N}(y | G(\theta), \Gamma(\phi))^\alpha p(\theta, \phi).$$

We assume that the covariance $\Gamma(\phi)$ is positive-definite for all $\phi$, and the prior $p(\theta, \phi)$ and posterior $\pi(\theta, \phi)$ are well-defined probability densities with full support over $\Theta \times \Phi$. Further, the prior can be written as $p(\theta)p(\phi | \theta)$ for $p(\theta)$ and $p(\phi | \theta)$ both well-defined density functions. In all of our numerical experiments in section 4, we use $\Gamma(\phi) = \phi I$, which is guaranteed to be positive-definite if $\phi$ is strictly positive. Given the dependence on $\phi$ in the covariance of the likelihood, note that the normalising constant is no longer $(\det (2\pi \Gamma))^{-1}$ as it is when the covariance is fully specified.

In order for the posterior to be well-defined, the likelihood $\mathcal{N}(y | G(\theta), \Gamma(\phi))$ must be integrable with respect to the prior $p(\phi)$ at the observed value of $y$, so that the posterior normalising constant exists (see theorem 2.5 of Latz (2020) and the surrounding discussion for further details). Such an assumption is implicitly maintained in any Bayesian analysis and is reasonable when using a conventional prior specification such as those maintained in section 4. Furthermore, if the normalising constant exists, and the likelihood is a continuous and strictly positive probability function that is uniformly bounded from above by an integrable function, then it can be shown that the solution given by the posterior is Hellinger, total variation and weakly well-posed (see theorem 3.6 of Latz (2020). Dunlop (2019) also shows well-posedness of the posterior for models with purely multiplicative noise and a mixture of additive and multiplicative noise. Given that the posterior is a well-defined probability density, the stability and performance of the algorithm is controlled through adaptation of the tempering parameter $\alpha_j$. As with IEKI, we use the approach of Jasra et al. (2010) to adapt $\alpha_j$, thereby ensuring that a prespecified ESS, with respect to the approximate target, is maintained when transitioning between the densities. Note also, that instability in the transitions between targets will be
reflected in the adapted tampering schedule $\alpha_1, \ldots, \alpha_j, \ldots, \alpha_{J-1}$, i.e. the estimated ESS will be low even for very small changes in $\alpha_j$.

At each iteration $j = 1, \ldots, J$, the model parameters $\theta$ and the noise parameters $\phi$ are updated component-wise conditional on the other. We refer to our method as CW-IEKI. Our proposed procedure for CW-IEKI is as follows:

1. Sample $\{\theta^n_0, \phi^n_0\} \sim p(\theta, \phi)$ for $n = 1, \ldots, N$.
2. Update the model parameters $\theta$: $\tilde{\theta}^n_j = \tilde{\theta}^n_j + \tilde{C}^n_j (\tilde{C}^n_j)(\tilde{\phi}^{n-1}_j)^{-1} (y_n - \tilde{y}^n_j)$ where $\tilde{\theta}^n_j = \theta^n_{j-1}$ and $\tilde{y}^n_j \sim N(G(\tilde{\theta}^n_j), (\alpha_j - \alpha_{j-1})^{-1} \Gamma(\theta^n_{j-1}))$ for $n = 1, \ldots, N$.
3. Update the noise parameters $\phi$: update $\phi^n_j$ conditional on $\theta^n_j$ for $n = 1, \ldots, N$ using the Metropolis–Hastings MCMC update shown in algorithm 1.
4. Iterate steps 2 and 3 until $\alpha_j = \alpha_J = 1$.

The covariance (8) in step 2 is

$$\tilde{C}^n_j (\phi^{n-1}_j) = \frac{1}{N-1} \sum_{n=1}^N \left( g^n_j - \frac{1}{N} \sum_{k=1}^N g^n_k \right) \left( g^n_j - \frac{1}{N} \sum_{k=1}^N g^n_k \right)^\top + \frac{1}{\alpha_j - \alpha_{j-1}} \Gamma (\phi^{n-1}_j).$$

The main innovation of our method is the inclusion of step 3. The IEKI update in step 2 requires fixed values of $\phi$, so a natural solution is to update $\theta$ conditional on $\phi$ (step 2), then update $\phi$ conditional on $\theta$ (step 3). MCMC is a convenient choice, as it allows $\phi$ to be updated according to its full conditional posterior distribution, $\pi(\phi \mid \theta)$, albeit conditioned on the biased samples of $\theta$ from step 2. If $\theta \sim \pi_j(\theta \mid \phi, y)$ after step 2 and the MCMC algorithm in step 3 is run to convergence, then the joint samples of $\theta$ and $\phi$ are distributed according to $\pi_j(\theta, \phi \mid y) \propto p(y \mid \theta, \phi)^\alpha p(\theta, \phi)$ as $N \to \infty$ (Del Moral et al. 2006). In general, however, $\theta$ is not updated according to $\pi_j(\theta \mid \phi, y)$ in CW-IEKI, even for linear Gaussian models. See section 3.1 for a more in-depth discussion of CW-IEKI.

For step 3, we propose to use $M$ iterations of a Metropolis–Hastings MCMC kernel, where the ensemble $\phi^{1:M}_j$ can be used to inform the proposal distribution for $\phi$. In our examples in sections 4.2–4.6, we use a random walk proposal of the form $q(\cdot \mid \phi^m_{j-1}) = N(\phi^m_{j-1}, \Sigma)$, for $n = 1, \ldots, N$, where $\Sigma$ is the covariance of the ensemble $\phi^{1:M}_j$. If it is possible to independently sample from $\pi_j(\phi \mid \theta)$, then Gibbs sampling can also be used to update $\phi^{1:M}_j$. Note that step 3 does not require evaluation of $G(\cdot)$ since $\theta$ is fixed. Consequently, the total number of evaluations of $G(\cdot)$ for our method is the same as for IEKI, i.e. $JN$, which again is typically much less than the $N\sum_{i=1}^J M_i + 1$ evaluations required for likelihood tempering SMC. See algorithm 1 for more details.

To adapt $\alpha_j$, the weights are calculated in a similar way to IEKI,

$$w^n_j = \frac{\pi_j (\phi^{n-1}_j, \theta^n_{j-1})}{\pi_{j-1} (\phi^{n-1}_j, \theta^n_{j-1})} \propto \exp\left( \log (\alpha_j - \alpha_{j-1}) - \frac{1}{2} \log \det \Gamma (\phi^{n-1}_j) - \frac{\alpha_j - \alpha_{j-1}}{2} (y - G(\theta^n_{j-1}))^\top \Gamma (\phi^{n-1}_j)^{-1} \right) \times \left( y - G(\theta^n_{j-1}) \right).$$
Set $\phi_m$ of $\tilde{\phi}$.

However, unlike standard fixed-point recursions, this recursion is stochastic due to simulation error arising from model misspecification as well as measurement error.

Similar to SMC, the IEKI algorithm of Iglesias (2014) produces a sequence of posteriors $\pi_0(\theta), \ldots, \pi_J(\theta)$ such that at the $J$th, and final, iteration of the algorithm the resulting posteriors draws should constitute a reasonable approximation to

$$\pi_J(\theta) \propto \mathcal{N}(y | G(\theta), \Gamma)^{\alpha_j} p(\theta).$$

In an attempt to understand the IEKI algorithms’ output, let us rewrite the step 2 of the IEKI algorithm as follows: for $y_f \sim \mathcal{N}(0, I)$ and $H_f = \tilde{C}_f (\tilde{C}_f^T)^{-1}$,

$$\begin{aligned}
\theta^n_j &= \theta_{n-1}^j + H_f \{y - \tilde{y}_f^n\} \\
&= \theta_{n-1}^j + H_f \{y - G(\theta_{n-1}^j) - (\alpha_j - \alpha_{j-1})^{-1} \Gamma \tilde{y}_f^n\}. 
\end{aligned}$$

Equation (11) clarifies that $\theta^n_j$ evolves according to what resembles a stochastic fixed-point recursion: for a given $n$, if at the $j$th iteration, $j > 1$, $\theta_{n-1}^j$ is such that $H_f \{y - G(\theta_{n-1}^j) - (\alpha_j - \alpha_{j-1})^{-1} \Gamma \tilde{y}_f^n\} = 0$, then the algorithm returns $\theta^n_j = \theta_{n-1}^j$ for every further value of $j$. However, unlike standard fixed-point recursions, this recursion is stochastic due to simulation of $\tilde{y}_f^n$ (i.e. $\tilde{y}_f^n$), which makes analysing its convergence properties difficult.

---

**Algorithm 1. MCMC update of the noise parameters $\phi$.**

**Input:** data $y$, ensembles $\theta_1^N$ and $\phi_1^N$, model evaluations $g^n = G(\theta_j^n)$ for all $n = 1, \ldots, N$ and $\alpha_j$

**Output:** updated ensemble of noise parameters $\phi_1^N$

Set $\phi_1^N = \phi_1^{1-N}$

for $n = 1$ to $N$ do

Sample $\phi_{n}^{*,*} \sim q(\cdot | \phi_{n}^*)$

Calculate the acceptance probability

$$\alpha(\phi_{n}^*, \phi_{n}^{*,*}) = \min \left( 1, \frac{\mathcal{N}(y | g_{\phi_{n}^{*,*}}, \Gamma_{\phi_{n}^{*,*}})}{\mathcal{N}(y | g_{\phi_{n}^*}, \Gamma_{\phi_{n}^*})} \frac{p(\theta_{n}^{*,*}, \phi_{n}^{*,*}) q(\phi_{n}^{*,*} | \phi_{n}^*)}{p(\theta_{n}^*, \phi_{n}^*) q(\phi_{n}^* | \phi_{n}^{*,*})} \right)$$

Sample $u \sim \text{Uniform}(0, 1)$

if $\alpha(\phi_{n}^*, \phi_{n}^{*,*}) < u$ then

Set $\phi_{n}^* = \phi_{n}^{*,*}$

end if

end for

These weights are normalised to give $W_1^{1-N}$, and $\alpha_j$ is adapted such that the ESS, estimated using (9), matches the target threshold.

Note that since $\phi$ is estimated in CW-IEKI, the likelihood covariance $\Gamma(\phi)$ may capture error arising from model misspecification as well as measurement error.

### 3.1. Discussion of IEKI and CW-IEKI

Similar to SMC, the IEKI algorithm of Iglesias (2014) produces a sequence of posteriors $\pi_0(\theta), \ldots, \pi_J(\theta)$ such that at the $J$th, and final, iteration of the algorithm the resulting posteriors draws should constitute a reasonable approximation to
Indeed, conditional on $\theta_{j-1}^n$, for each $n = 1, \ldots, N$, and fixed $j$, equation (11) clarifies that step 2 of the IEKI algorithm can be seen as producing a draw, $\theta_j^n$, from the distribution

$$
\theta \mid y, \theta_{j-1}^n \sim N \left( \theta_{j-1}^n + \tilde{H}_j^n \left\{ y - G \left( \theta_{j-1}^n \right) \right\}, (\alpha_j - \alpha_{j-1})^{-1} \tilde{H}_j^n \Gamma \left( \tilde{H}_j^n \right)^{-1} \right).
$$

Note that, for any finite $N$ and $J$, the above is not a draw from $\pi_J(\theta)$. Moreover, given the recursive, and stochastic, nature of the algorithm, establishing convergence of the original IEKI algorithm, or precisely what distribution it converges towards, is no simple task.

To our knowledge, there does not exist a precise analysis of the theoretical properties of the posterior produced via the IEKI algorithm in our specific context. Existing results on the behavior of the IEKI algorithm mostly rely on a continuous limit approximation of the iterates (see, e.g. Blömker et al. 2018, 2019, and Blömker et al. 2021), which allows one to leverage the resulting continuous time stochastic differential equations that underlie the limit version of the algorithm. However, such analysis abstracts away from the finite nature of the iteration scheme, and thus does not necessarily produce interpretable results on the IEKI posterior.

The above discussion can also be used to help us understand the output of the CW-IEKI algorithm. In particular, now letting $\Gamma = \Gamma(\phi)$, and conditional on $\tilde{y}_j^m$ and $\phi_j^n$, step 2 of the CW-IEKI algorithm (the $\theta$-step) can be characterised as

$$
\theta_j^n = \theta_{j-1}^n + \tilde{H}_j^n \left( \phi_j^n \right) \left\{ y - G \left( \theta_{j-1}^n \right) - (\alpha_j - \alpha_{j-1})^{-1} \Gamma \left( \phi_j^n \right) \tilde{y}_j^n \right\}, \quad (12)
$$

where $\tilde{H}_j^n(\phi_j^n) = \tilde{C}_j^n \left( \phi_j^n \right)^{-1} \tilde{C}_j^n(\phi_j^n)$. Unsurprisingly, equation (12) reveals that the $\theta$-step of CW-IEKI algorithm updating scheme has now been further complicated by its (possibly non-linear) dependence on $\phi_j^n$.

The introduction of the sampling step for $\phi_j^n$ in the CW-IEKI algorithm further complicates theoretical analysis of the algorithm. Recall that before moving onto the MCMC sampling step for $\phi_j^n$, we have already updated $\theta_j^n$ from equation (12), which requires simulation of $\tilde{y}_j^n$ (through $\tilde{y}_j^n$). Thus, the acceptance probability $\alpha(\phi_j^n, \phi_j^{n*})$ calculated in algorithm 1 depends on the simulated realisation of $\tilde{y}_j^n$, where $\tilde{y}_j^n \sim N(0, I)$; see equation (12).

Consequently, the output of the MCMC step in the CW-IEKI algorithm is the output of a pseudo-marginal sampling scheme (Andrieu and Roberts 2009), i.e. an MCMC scheme where the acceptance probability relies on simulated variables. See Martin et al. (2020) for a brief overview of pseudo-marginal methods. In general, when the acceptance probability $\alpha(\phi_j^n, \phi_j^{n*})$ depends on simulated variables, say $\tilde{y}$, the accepted draw $\phi_j^n$ is not obtained from a target distribution based solely on $\phi$, but is obtained from a joint distribution for $\phi$ and $\tilde{y}$. Critically, unless the resulting likelihood terms in the acceptance probability $\alpha(\phi_j^n, \phi_j^{n*})$ are unbiased estimators, even upon convergence of the MCMC chain the marginal accepted draw $\phi_j^n$ will not be from the appropriate marginal distribution (Andrieu and Roberts 2009). That is, while the results of Andrieu and Roberts (2009) suggest that the posterior distribution from the CW-IEKI algorithm is well-defined, the resulting posterior will in general differ from $\pi_J(\theta, \phi)$ unless we are employing an unbiased estimator of the likelihood $N(y \mid G(\theta), \Gamma(\phi))$ within the algorithm.

In the MCMC step in algorithm 1, the likelihood term is $N(y \mid G(\theta_j^n), \Gamma(\phi_j^n))$, and, by equation (12) we see that $G(\theta_j^n)$ depends on the simulated random variable $\tilde{y}_j^n$. Moreover, by Jensen’s inequality

$$
E_{\tilde{y}} \left[ N \left( y \mid G(\theta_j^n), \Gamma(\phi_j^n) \right) \right] \geq N \left( y \mid E_{\tilde{y}} \left[ G(\theta_j^n) \right], \Gamma(\phi_j^n) \right).
$$
Consequently, even upon convergence of the algorithm there is no reason to suspect that the CW-IEKI algorithm will deliver samples from the target posterior \( \pi_j(\theta, \phi) \propto N(y | G(\theta), \Gamma(\phi))^{\alpha_j} p(\theta, \phi) \).

While both the IEKI and CW-IEKI algorithms are difficult to analyse theoretically, this does not diminish their practical relevance, and as we shall see shortly the CW-IEKI algorithm performs well across several applications. Given this, we believe a formal study on the CW-IEKI algorithm is warranted, however, we maintain that such an analysis is beyond the scope of this current article.

4. Performance of CW-IEKI

4.1. Implementation of CW-IEKI and likelihood tempering SMC

We compare CW-IEKI to likelihood tempering SMC on five examples. The first is a univariate linear Gaussian model, and the second is a set of non-linear population models applied to simulated data. The third example is a model of nitrogen mineralisation in soil (Vilas et al. 2021) that has relatively few parameters. The fourth example predicts seagrass decline due to cumulative water temperature and light stress (Adams et al. 2020), and the fifth and final example predicts coral calcification rates (Galli and Solidoro 2018). The seagrass model has more parameters than the first three examples, and its marginal posteriors are roughly Gaussian. The coral model also has a relatively large number of parameters, but relatively uninformative data—only a few directions in the parameter space are informed by the data. Except for the linear Gaussian model, all model examples have a mean governed by non-linear dynamics, and use a non-Gaussian prior. Additionally, while the likelihood of the population, nitrogen mineralisation and coral models are Gaussian, the likelihood of the seagrass model is close to, but not strictly, Gaussian. See section 4.5 for more detail on the likelihood function of the seagrass model.

Following Iglesias et al. (2018), we compare our novel method to SMC as the gold standard since it is exact as the number of particles \( N \to \infty \) and our new approximate method aims to mimic its algorithmic structure. All code is implemented in MATLAB. For both CW-IEKI and SMC, the ensemble size is fixed at 1000, and the tempering parameter \( \alpha_j \) is adapted to achieve a target ESS of \( N/2 = 500 \) unless otherwise specified. To mutate the noise ensemble \( (\phi^j_{1:N}) \) in CW-IEKI and the particles \( \{\theta, \phi\}^j_{1:N} \) in SMC we use a random walk Metropolis–Hastings kernel (Hastings 1970), where the covariance of the random walk proposal is set to the covariance of the samples being mutated, i.e. \( \text{cov}(\phi^j_{1:N}) \) for CW-IEKI and \( \text{cov}(\{\theta, \phi\}^j_{1:N}) \) for SMC. Due to the higher number of parameters for the seagrass and coral models, the covariance of the random walk is scaled by \( 2^{38^2/(d_\theta + d_\phi)} \) for SMC, where \( d_\theta \) is the number of parameters in \( \theta \) and \( d_\phi \) is the number of parameters in \( \phi \) (Roberts and Rosenthal 2001). For CW-IEKI, the number of MCMC iterations is fixed at a conservative 1000—as no extra model evaluations are required, the cost of these iterations is relatively small. For SMC, the number of MCMC iterations is adapted at each iteration \( j = 1, \ldots, J \) as follows (South et al. 2019):

1. Run \( S_j \) MCMC iterations and estimate the acceptance rate \( p \).
2. Adapt the total number of MCMC iterations as \( M_j = \lceil \log(1/c)/\log(1 - p) \rceil \).
3. Complete the remaining \( M_j - S_j \) MCMC iterations.
4. Calculate \( S_{j+1} \) for the next iteration as \( S_{j+1} = \lfloor M_j/2 \rfloor \).

Here \( p \) is the estimated MCMC acceptance rate based on all the particles, i.e. the proportion of acceptances out of \( N \times S_j \) MCMC trials. Here \( 1 - c \) denotes the theoretical probability
of moving each SMC particle at least once in the $M_j$ MCMC iterations. To encourage high diversity in the SMC population, we set $c$ to be small, specifically $c = 0.01$. For ease of exposition, assume $M_j = M$ for $j = 1, \ldots, J$. The value of $M$ largely determines the computational cost of SMC, in terms of the number of evaluations of the function $G(\cdot)$. However, if the value of $M$ is too low, the resulting set of samples will not be a good representation of the posterior distribution. Furthermore, a good value of $M$ is highly model and application specific. As a result, the value of $M$ is generally adapted in practice (South et al 2019) as it bypasses the need for a potentially expensive tuning step, for example, using pilot runs of SMC.

We assess the performance of CW-IEKI based on its accuracy, predictive performance and computation time relative to SMC. The marginal posterior density plots of the model parameters are used to compare the accuracy of CW-IEKI to the SMC solution. As these plots do not account for parameter interdependencies however, we also compare the marginal densities of parameter combinations that greatly influence the model fit (Monsalve-Bravo et al 2022). These combinations are identified through the eigendecomposition of a sensitivity matrix that captures key characteristics of the posterior distribution. Unless otherwise specified, we calculate the sensitivity matrix as the inverse of the sample covariance of the natural logarithm of the posterior samples from SMC (Monsalve-Bravo et al 2022). The logarithm of the $k$th parameter combination is

$$\alpha_k = \sum_{j=1}^{d_\theta} (v_k)_j \log \theta_j,$$

where $(v_k)_j$ is the $j$th element of the $k$th normalised eigenvector, and $\theta_j$ is the $j$th parameter. Following the terminology of Monsalve-Bravo et al (2022), we refer to (13) as the logarithm of the $k$th eigenparameter. The stiffest and sloppiest eigenparameters are those associated with the highest and lowest eigenvalues, respectively. For all examples, the noise parameters $\phi$ are treated as nuisance parameters in the analysis of model sloppiness and are excluded when calculating the sensitivity matrix (Monsalve-Bravo et al 2022).

Posterior predictive plots are used to assess the predictive performance of CW-IEKI relative to SMC. The posterior predictive distribution is given by

$$p(y^* | y_{1:T}) = \int_\Theta p(y^* | \theta) p(\theta | y_{1:T}) d\theta,$$

which can be sampled for $n = 1, \ldots, N$ as follows:

(1) Sample from the posterior distribution $\{\theta, \phi\}_n^* \sim p(\cdot | y_{1:T})$.
(2) Sample from the likelihood $y_n^* | \{\theta, \phi\}_n^* \sim \mathcal{N}(\cdot | G(\theta_n^*), \Gamma(\phi_n^*))$.

Since it is generally not possible to sample from the posterior distribution directly, a sampling method may be used in step 1. Note that if the samples from step 1 are from an approximation to the posterior, the sampled predictions will be from an approximation to the posterior predictive distribution. We compare the posterior predictive distribution estimated using the biased posterior samples from CW-IEKI to the posterior predictive distribution using the asymptotically exact samples from SMC.

Since SMC is asymptotically exact, it is always expected to outperform CW-IEKI in terms of accuracy and predictive performance. Note, however, that the output from CW-IEKI will not necessarily be Gaussian. While the updates of the samples are linear Gaussian at each iteration, the coefficients of the updates evolve non-linearly. See the proof of theorem 2.1 and
Figure 1. Marginal posterior densities for $b$ and $\sigma$ for the linear Gaussian model. Models were fitted using SMC (blue), CW-IEKI (red-orange) and IEKI with $\sigma$ fixed at 0.5 (yellow), 0.25 (purple) and 1 (green).

remark 2.2 in Iglesias et al (2013). Therefore, for non-linear models we would generally expect non-Gaussian posteriors.

The main advantage of CW-IEKI is a significant speed-up in computation time compared to SMC. We assume that the expense of evaluating the function $G(\cdot)$, i.e. the deterministic mean of the likelihood function, dominates the computation time. SMC has $N\sum_{j=1}^J M_j + 1$ evaluations of $G(\cdot)$, while CW-IEKI only has $NJ$. The value of $N$ is fixed for both methods, while $J$ and $M_j, j = 1, \ldots, J$ are adapted. In general, $\sum_{j=1}^J M_j + 1 \gg J$, especially as the dimension of the parameter space increases. In particular, since the acceptance rate for the Metropolis–Hastings algorithm generally decreases with increasing dimension of the parameter space (Roberts and Rosenthal 2001), $M_j$ for $j = 1, \ldots, J$ should scale with the dimension of the problem to ensure sufficient movement of the particles at each iteration of SMC.

4.2. Example 1: univariate linear Gaussian model

Here we demonstrate improved performance of CW-IEKI compared to IEKI when $\phi$ is unknown using an illustrative example

$$y \sim \mathcal{N}(b \cdot 1, \sigma^2 \cdot I),$$

where $b$ and $\sigma$ are unknown, $1$ is a vector of length $d_y$ containing all ones, and $I$ is the identity matrix of size $d_y \times d_y$. We simulate $d_y = 50$ observations from equation (14) with $b = 0.5$ and $\sigma = 0.5$. The priors for $b$ and $\sigma$ are $\mathcal{N}(b \mid 0.5, 1)$ and $\mathcal{N}(\log(\sigma) \mid 1, 1)$. Since $\sigma$ is constrained to be positive, a log-transformation is used to allow for sampling over an unconstrained space.

We run the IEKI method of Iglesias et al (2018) with $\sigma$ fixed at 0.5 (the ‘true’ value), 0.25 and 1. IEKI with $\sigma$ fixed at the true value is included for reference only, as the exact covariance of the noise is rarely known in practice. Figure 1 shows the marginal posterior densities of $b$ and $\sigma$ from all methods, and table 1 shows the computation cost.

Based on the marginal posterior densities, CW-IEKI outperforms IEKI when $\sigma$ is misspecified ($\sigma = 1$ or $\sigma = 0.25$), and it correctly identifies $\sigma$ values with high posterior support, although with a heavier right tail. While figure 1 shows that CW-IEKI is not exact for linear Gaussian models, i.e. the marginal posterior densities from the CW-IEKI samples are not the same as those from the SMC samples, this is also true for IEKI when the covariance is misspecified. Unsurprisingly, IEKI outperforms CW-IEKI when the true value of $\sigma$ is known—CW-IEKI assumes that $\sigma$ is unknown, and no information on $\sigma$ was included in the CW-IEKI run. All IEKI based methods have significantly fewer evaluations of $G(\cdot)$ compared to SMC, with 2000–6000 evaluations compared to the 58000 from SMC.
For our second example, we consider the following population models from Peters et al (2010) for \( t = 1, \ldots, 50 \).

(1) Ricker: \( \log (y_t) \sim \mathcal{N}(\beta_0 + \log(y_{t-1}) + \beta_1 y_{t-1}, \sigma^2) \).
(2) Theta-logistic: \( \log (y_t) \sim \mathcal{N}(\beta_0 + \log(y_{t-1}) + \beta_1 y_{t-1}, \sigma^2) \).
(3) Flexible-allee: \( \log (y_t) \sim \mathcal{N}(\beta_0 + \log(y_{t-1}) + \beta_1 y_{t-1} + \beta_3 y_{t-1}^2, \sigma^2) \).
(4) Mate-limited: \( \log (y_t) \sim \mathcal{N}(\beta_0 + 2\log(y_{t-1}) + \beta_1 y_{t-1} - \log(\beta_4 + y_{t-1}), \sigma^2) \).

Data was simulated from the Ricker model using \( \log (y_0) = 2, \sigma = 1 \) and \( \theta = \{\beta_0, \beta_1\} = \{2, -0.5\} \), which corresponds to \( \theta = \{\beta_0, \beta_1, \beta_2\} = \{2, -0.5, 1\} \) for the theta-logistic model, \( \theta = \{\beta_0, \beta_1, \beta_3\} = \{2, -0.5, 0\} \) for the flexible-allee model and \( \theta = \{\beta_0, \beta_1, \beta_4\} = \{2, -0.5, 0\} \) for the mate-limited model. All models are calibrated to the same dataset. The priors used are \( \beta_0 \sim \mathcal{N}(1,1), \beta_2 \sim \mathcal{N}(1,0.25), \beta_1, \beta_3 \sim \mathcal{N}(0,1) \) and \( \beta_4, \sigma \sim \text{Half-Normal}(1) \).

As with the linear Gaussian model example in section 4.2, we run SMC, CW-IEKI and the IEKI method of Iglesias et al (2018) with \( \sigma \) fixed at 1 (the ‘true’ value), 0.5 and 2. Results are shown in table 2 and figure 2. Due to the chaotic nature of the model, the posterior predictive distribution is not shown—the predictions range from 0 to infinity even for the samples from SMC. For all models, CW-IEKI has fairly good performance compared to SMC and out-performs IEKI when \( \sigma \) is misspecified. Interestingly, for the mate-limited model CW-IEKI
Figure 2. Marginal posterior density plots of the parameters from the four models. Samples are obtained using SMC (blue), CW-IEKI (red-orange) and IEKI with $\sigma$ fixed at 1 (yellow), 0.5 (purple) and 2 (green). Note that the true value of $\beta_4$ is 0.

outperforms IEKI even when $\sigma$ is correctly specified. Again, the IEKI based methods are significantly faster than SMC, with CW-IEKI having 12 to 16 times fewer evaluations of $G(\cdot)$ compared to SMC.
4.4. Example 3: predicting nitrogen mineralisation

The third model predicts cumulative nitrogen mineralisation (CNM), assuming a measurement error distributed according to (Vilas et al 2021):

\[ y'_j \sim \mathcal{N}(x_j, (\zeta'_j)^2 + \sigma^2), \quad x_j = G(\theta, t_j), \]

for \( j = 1, \ldots, T \) and \( r = 1, \ldots, R \), where \( T \) is the number of timepoints, \( R \) is the number of replicates per timepoint, and \( x_1, \ldots, x_T \) are deterministic predictions of CNM from version 7.10 of the APSIM model (Holzworth et al 2014) configured with soil water and nitrogen modules (Probert et al 1998). The function \( G(\cdot) \) has numerous parameters, most of which are fixed at measured values (Probert et al 1998), apart from the model parameters we seek to obtain improved estimates for. Following the approach of Ramnay et al (2020), the model error is separated into two parts, where the first term \( (\zeta'_j) \) is known and accounts for measurement error, and the second term \( (\sigma) \) is unknown and accounts for all other sources of error such as model misspecification. At each timepoint \( t_j, j = 1, \ldots, T \) and replicate \( r = 1, \ldots, R \), \( \zeta'_j \) is set to 4% of the observation \( y'_j \) (APHA and AWWA 2012).

We consider two versions of this model. The first estimates three parameters (biom, finert, \( \sigma \)) and is the one considered in Vilas et al (2021). For the second model, three additional model parameters are estimated (\( \text{ef\_biom} = \text{ef\_hum}, \text{rd\_biom} \) and \( \text{rd\_hum} \))—in the first model these parameters are fixed at \( \text{ef\_biom} = \text{ef\_hum} = 0.4, \text{rd\_biom} = 0.0081 \) and \( \text{rd\_hum} = 0.00015 \). As a shorthand, in the present work we refer to these two models as the three parameter and six parameter APSIM models respectively. See Probert et al (1998) for more detail about the model parameters and the values of the remaining parameters. The models are applied to data from Allen et al (2019) measuring changes in inorganic nitrogen in soil from the Mackay Whitsundays region of North Queensland. The data is obtained from four 301 day laboratory incubations (i.e. \( R = 4 \)). The second model is also fitted to a dataset simulated using \( \theta = \{ \text{biom, finert, ef\_biom = ef\_hum, rd\_biom, rd\_hum} \} = \{0.1, 0.6, 0.3, 0.0025, 0.0005 \} \) and \( \phi = \sigma = 8 \). To enable simulation from the model, the known portion of the error \( (\zeta'_j) \) is set to 4% of the mean at time \( t_j \), i.e. for the synthetic dataset, \( \zeta'_j = 0.04 \cdot x_j \), for all \( r = 1, \ldots, 4 \), matching the number of replicates in the data from Allen et al (2019).

We denote the truncated univariate normal distribution as \( \mathcal{N}(x \mid \mu, \sigma^2, a, b) \), where \( \mu \) is the mean, \( \sigma \) is the standard deviation, \( a \) is the lower bound, and \( b \) is the upper bound. The assumed priors for biom, finert and \( \sigma \) are \( \mathcal{N}(\text{biom} \mid 0.093, 0.025^2, 0.05, 0.15) \), \( \mathcal{N}(\text{finert} \mid 0.58, 0.1^2, 0.4, 0.8) \) and Uniform(\( \sigma \mid 0, 20 \)) for both models. For the second model, the additional priors are Uniform(\( \text{ef\_biom} = \text{ef\_hum} \mid 0, 1 \)), Uniform(\( \text{rd\_biom} \mid 0.001, 0.01 \)) and Uniform(\( \text{rd\_hum} \mid 0, 0.001 \)).

4.4.1. Three parameter APSIM model applied to the real data. Figure 3 shows the marginal posterior densities of the parameters and the eigenparameters of the three parameter APSIM model applied to the real data. Figure 3 also shows the posterior predictive densities using CW-IEKI and SMC. On this example, both CW-IEKI and SMC have very similar results for accuracy and predictive performance. However, CW-IEKI is more than five times faster than SMC with 10000 evaluations of \( G(\cdot) \) compared to 54000 for SMC. (The number of evaluations of \( G(\cdot) \) in our study is always a multiple of 1000 because our chosen ensemble sizes for both CW-IEKI and SMC are \( N = 1000 \).)
Figure 3. Marginal posterior density plots of the parameters (top row) and the natural logarithm of the eigenparameters (middle row), as well as a comparison of the real data to the median and 95% central credible intervals for the posterior predictive distribution of cumulative nitrogen mineralisation (CNM; bottom row) obtained from the three parameter APSIM model fitted to the real data. Note that the uncertainty parameter $\sigma$ is excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (13). The eigenparameter results are based on the prior (black), CW-IEKI (red-orange) and SMC (blue) using a sensitivity matrix calculated using the SMC samples.

4.4.2. Six parameter APSIM model applied to the real data. Figure 4 shows the marginal posterior density plots of the parameters and the three stiffest eigenparameters of the six parameter APSIM model applied to the real data. Figure 4 also shows the posterior predictive densities, and figure 5 shows the eigenvectors of the three stiffest eigenparameters. Unlike the three parameter model, the CW-IEKI and SMC marginal posterior densities have different means for some of the parameters. The predictive performance of CW-IEKI and SMC are relatively similar for this example however, except that the CW-IEKI results have greater uncertainty. This is also shown in the marginal posterior for $\sigma$, where CW-IEKI retains larger values of $\sigma$ in its posterior approximation compared to SMC.

Based on the eigenvectors in figure 5, the parameters $ef_{biom} = ef_{hum}$ and rd_hum do not contribute significantly to the model fit. Interestingly, the CW-IEKI marginal posteriors for these two parameters show the greatest bias compared to the SMC results. Overall, CW-IEKI gives a reasonably good fit for the model. CW-IEKI is also around 33 times faster than SMC with 9000 evaluations of $G(\cdot)$ compared to 301000.
4.4.3. *Six parameter APSIM model applied to the simulated data.* Figure 6 shows the marginal posterior densities of the six parameter APSIM model applied to the simulated data. As before, SMC and CW-IEKI have similar results, except that CW-IEKI has posterior support for larger values of $\sigma$. Figures 6 and 7 show the densities and eigenvectors of the three stiffest eigenparameters respectively. The eigenparameter densities are very similar for SMC and CW-IEKI, indicating that CW-IEKI gives a relatively good fit for the model, and the eigenvectors again show that $\text{ef}_{\text{biom}} = \text{ef}_{\text{hum}}$ and $\text{rd}_{\text{hum}}$ have little influence on the model fit. The posterior predictive distribution in figure 6 also shows similar performance between SMC and CW-IEKI, except that CW-IEKI has much greater uncertainty. On this example, CW-IEKI is around 37 times faster than SMC with 11000 evaluations of $G(\cdot)$ compared to 411 000.
Figure 5. Eigenvectors of the three stiffest eigenparameters for the six parameter APSIM model applied to the real data. These results are based on the SMC posterior samples. The labels on the left-hand side correspond to $v_k(\lambda_k/\lambda_1)$, where $v_k$ and $\lambda_k$ are the eigenvector and associated eigenvalue of eigenparameter $k$, respectively. The shade of the cells in row $k$ indicates the relative contribution ($v_k$) of the $j$th parameter to eigenparameter $k$—parameters with darker colours have the greatest contribution.

Figure 6. Marginal posterior density plots of the parameters (top row) and the natural logarithm of the eigenparameters (middle row), as well as a comparison of the simulated data to the median and 95% central credible intervals for the posterior predictive distribution of cumulative nitrogen mineralisation (CNM; bottom row) obtained from the six parameter APSIM model fitted to the simulated data. Note that the uncertainty parameter $\sigma$ is excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (13). The eigenparameter results are based on the prior (black), CW-IKEI (red-orange) and SMC (blue) using a sensitivity matrix calculated using the SMC samples.
Figure 7. Eigenvectors of the three stiffest eigenparameters for the six parameter APSIM model applied to the simulated data. These results are based on the SMC posterior samples. The labels on the left-hand side correspond to $v_k(\lambda_k/\lambda_1)$, where $v_k$ and $\lambda_k$ are the eigenvector and associated eigenvalue of eigenparameter $k$, respectively. The shade of the cells in row $k$ indicate the relative contribution ($v_k$) of the $j$th parameter to eigenparameter $k$—parameters with darker colours have the greatest contribution.

4.5. Example 4: predicting seagrass decline

The fourth model predicts shoot density decline in seagrass due to cumulative stress from water temperature and light (Adams et al. 2020). The model takes, as input, light, temperature and time period of stress, and outputs photosynthesis rates and changes in shoot density over time. The model has 18 model parameters and five noise parameters. Several of these parameters have different values for specific instantaneous temperatures $T$ and mean daily temperatures $\overline{T}$ (see Adams et al. 2020, for full model and parameter details). Uniform priors are used for all parameters. See table 1 for the parameter units and prior bounds.

The model is calibrated to net photosynthesis data (Collier et al. 2018) and shoot density data (Collier et al. 2016) separately for three species of tropical seagrass from the great barrier reef—Cymodocea serrulata, Halodule uninervis and Zostera muelleri. In the likelihood function for model-data calibration it is assumed that measurement noise present in net photosynthesis observations at a given temperature $T$ are normally distributed with standard deviation $\sigma_P(T)$. Similarly, measurement noise in shoot density observations is assumed to be normally distributed with standard deviation $\sigma_S$ (albeit with some modifications to account for when observed shoot density declines to zero, see appendix B of Adams et al. 2020 for further details).

For brevity, all results shown in this section are for $C. serrulata$. Results for $H. uninervis$ and $Z. muelleri$ are provided in appendix B. On this model, we also test the impact of the target ESS threshold on the accuracy of CW-IEKI. Figure 8 shows the marginal posterior densities of the parameters for SMC and CW-IEKI with the different ESS targets. For the majority of the parameters, the SMC and CW-IEKI densities are very similar. The target ESS threshold therefore appears to have little impact on the results.

As the parameters $\mu_{\text{net,max}}(21.9)$ and $\mu_{\text{net,max}}(27.9)$ are bounded between $-0.02$ and 0.02 (see table 3), the log-transform cannot be used when performing the analysis of model sloppiness. Instead, we rescale all the model parameter to be between $[0, 1]$ using the prior bounds, and then apply a logit transformation to map these values back to $[-\infty, \infty]$. The sensitivity matrix is given by the inverse of the covariance of the logit-transformed posterior samples from SMC, and the eigenparameters are given by

$$\alpha_k = \sum_{j=1}^{d_0} (v_k)_j \log \left( \frac{\hat{\theta}_j}{1 - \hat{\theta}_j} \right), \quad \hat{\theta}_j = \frac{(\theta_j - a_j)}{(b_j - a_j)}, \quad (15)$$
where \((v_k)_j\) is the \(j\)th element of the \(k\)th normalised eigenvector, \(\theta_j\) is the \(j\)th parameter, \(a_j\) is the prior lower bound of parameter \(j\) and \(b_j\) is the prior upper bound of parameter \(j\). Figures 9 and 10 show the marginal densities and eigenvectors of the six stiffest eigenparameters. The densities of these eigenparameters are similar for SMC and CW-IEKI, although again, the CW-IEKI results have greater uncertainty. Based on the eigenvectors in figure 10, the parameters \(\mu_{\text{net, max}}(21.9)\), \(\mu_{\text{net, max}}(27.9)\), \(C_{\text{other loss}}(21.9)\) and \(C_{\text{other loss}}(27.9)\) do not significantly influence the model fit. As with the six parameter APSIM model, the CW-IEKI marginal posteriors for less influential parameters show the greatest bias.

Figure 11 shows the posterior predictive plots of the net carbon fixation using SMC and CW-IEKI with an ESS target of 50%, and figure 12 shows the posterior predictive plots of the shoot density decline. The predictive performance of SMC and CW-IEKI are fairly similar for this example, except that the CW-IEKI predictions have greater uncertainty. As with the density plots, there is little difference between the posterior predictive plots for an ESS target threshold of 50% and higher ESS targets (not shown). Table 4 shows the computation cost for

![Figure 8. Marginal posterior density plots for the seagrass model applied to the C. serrulata data.](image-url)
Table 3. Units and prior bounds of all 23 parameters of the seagrass model. The noise parameters are $\phi = \{\sigma_P(21), \sigma_P(25), \sigma_P(30), \sigma_P(35), \sigma_S\}$, and $\theta$ is comprised of the remaining parameters. In the final column, Cs, Hu and Zm refers to the species C. serrulata, H. uninervis and Z. muelleri respectively. Single values represent the upper bound for all three seagrass species.

| Parameter | Unit | Temperatures (°C) | Lower bound (Zm, Cs, Hu) | Upper bound (Zm, Cs, Hu) |
|-----------|------|-------------------|--------------------------|--------------------------|
| $\mu_{\text{net}, \text{max}}(T)$ | d$^{-1}$ | $T \in \{21.9, 27.9\}$ | 0.02 | 0.02 |
| $C_{\text{other loss}}(T)$ | mg C g$^{-1}$ DW h$^{-1}$ | $T \in \{21.9, 27.9\}$ | 0 | 2.5 |
| $I_s(T)$ | $\mu$mol m$^{-2}$ s$^{-1}$ | $T \in \{21, 25, 30, 35\}$ | 0 | 1000 |
| $R(T)$ | mg C g$^{-1}$ DW h$^{-1}$ | $T \in \{21, 25, 30, 35\}$ | 0 | 2.5 |
| $P_{\text{max}}(T)$ | mg C g$^{-1}$ DW h$^{-1}$ | $T \in \{21, 25, 30, 35\}$ | 20 | 10, 10 |
| $\sigma_P(T)$ | mg C g$^{-1}$ DW h$^{-1}$ | $T \in \{21, 25, 30, 35\}$ | 0 | 2.5 |
| $k$ | d$^{-1}$/ mg C g$^{-1}$ DW h$^{-1}$ | $T \in \{21, 25, 30, 35\}$ | 0 | 0.05 |
| $S_0$ | shoots/pot | — | 0 | 100, 20, 50 |
| $\sigma_S$ | shoots/pot | — | 0 | 20 |

Figure 9. Marginal density plots of the six stiffest eigenparameters (calculated using equation (15)) for the seagrass model applied to the C. serrulata data. Note that the uncertainty parameters in $\phi$ are excluded from the analysis of sloppiness, and $\lambda_i$ is the eigenvalue associated with eigenvector $v_i$ in equation (15). The eigenparameters are calculated based on samples from the prior (black), CW-IEKI (dashed) and SMC (blue) using a sensitivity matrix calculated using the SMC samples.

SMC and CW-IEKI. For an ESS target of 50%, CW-IEKI is approximately 40 times faster than SMC.

The results suggest that CW-IEKI gives a good fit for predicting shoot density decline and carbon fixation for C. serrulata. CW-IEKI also gives a good fit for H. uninervis, but not for Z. muelleri (see appendix B). The relatively poor fit for the latter may be a result of the likelihood not being strictly Gaussian due to the modifications that ensure the predicted shoot density remains greater than or equal to 0. As a result of these modifications, the likelihood function is close to Gaussian for higher shoot density values, but deviates strongly when the shoot density declines to 0, which is more often the case for Z. muelleri than for the other seagrass species.
4.6. Example 5: predicting coral calcification rates

The final model predicts coral calcification rates by simulating the transport and reaction of relevant chemical species and metabolic fluxes from seawater to the coral skeleton. It is assumed that there are two layers between the seawater and the coral skeleton: the coelenteron and the extracellular calcifying medium (ECM).

The main reactions considered are photosynthesis and respiration (seawater ↔ coelenteron), passive transport processes (seawater ↔ coelenteron ↔ ECM), membrane transport processes (coelenteron ↔ ECM) and aragonite precipitation and dissolution (ECM ↔ coral skeleton). The two membrane transport pumps modelled as part of the membrane transport processes are a Ca-ATPase pump and a bicarbonate anion transport pump.
**Figure 12.** Comparison of the *C. serrulata* data to the median and 95% central credible intervals for the posterior predictive distribution of shoot density obtained from the seagrass model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). SI = surface irradiance and ‘hot’ or ‘cold’ indicates the temperature conditions under which the seagrass data was collected (Adams et al 2020).

**Table 4.** Total and relative number of evaluations of $G(\cdot)$ for SMC and CW-IEKI with different ESS target thresholds. Results are for the seagrass model applied to the *C. serrulata* data. Note that the total number of evaluations of $G(\cdot)$ is a multiple of the number of samples $N = 1000$.

| Method       | SMC   | CW-IEKI |
|--------------|-------|---------|
| ESS target threshold | 50%   | 95%     | 90%     | 80%     | 70%     | 60%     | 50%     |
| $G(\cdot)$ evaluations | 799 000 | 87 000  | 60 000 | 39 000 | 30 000 | 24 000 | 20 000 |
| Approximate speed-up | 1.00 | 9.18 | 13.32 | 20.49 | 26.63 | 33.29 | 39.95 |

The reactions are modelled by a system of ordinary differential equations (ODEs), and measurement error is assumed to be Gaussian with standard deviation $\sigma$. The calcification rate predictions of the model are obtained from the steady state solution of the ODEs—these are
Table 5. Units and prior bounds of all 21 parameters of the coral calcification model. For this model, the uncertainty parameter is $\phi = \sigma$.

| Reaction                  | Parameter | Unit     | Lower bound | Upper bound |
|---------------------------|-----------|----------|-------------|-------------|
| Passive transport processes| $k_{CO_2}$ | cm s$^{-1}$ | 0           | 0.1         |
|                           | $k_{pp}$  | cm s$^{-1}$ | 0           | 0.1         |
|                           | $s$       | cm s$^{-1}$ | 0           | 0.1         |
| Ca-ATPase mechanism       | $\alpha$  | —        | 0           | 1           |
|                           | $\beta$   | —        | 0           | 1           |
|                           | $v_M$     | cm s$^{-1}$ | 0           | 250         |
|                           | $E_0_c$   | $\mu$mol cm$^{-2}$ | 0           | $1.2 \times 10^7$ |
|                           | $k_{1c}$  | cm$^4$ s $\mu$mol$^{-2}$ | 0           | $1.4 \times 10^{-4}$ |
|                           | $k_{2c}$  | s$^{-1}$  | 0           | 0.5         |
|                           | $k_{3c}$  | s$^{-1}$  | 0           | 800         |
|                           | $k_{1b}$  | cm$^2$ $\mu$mol$^{-1}$ | 0           | 8           |
|                           | $k_{2b}$  | s$^{-1}$  | 0           | 500         |
|                           | $k_{3b}$  | cm$^3$ s $\mu$mol$^{-2}$ | 0           | $1 \times 10^{-7}$ |
| BAT mechanism             | $E_0_b$   | $\mu$mol cm$^{-2}$ | 0           | 1500        |
|                           | $k_{1b}$  | cm$^3$ $\mu$mol$^{-1}$ s$^{-1}$ | 0           | $5 \times 10^{-5}$ |
|                           | $k_{2b}$  | s$^{-1}$  | 0           | 0.01        |
|                           | $k_{3b}$  | s$^{-1}$  | 0           | 0.01        |
|                           | $k_{1b}$  | s$^{-1}$  | 0           | $2 \times 10^{-4}$ |
|                           | $k_{2b}$  | s$^{-1}$  | 0           | $1 \times 10^{-3}$ |
|                           | $k_{3b}$  | cm$^3$ $\mu$mol$^{-1}$ s$^{-1}$ | 0           | $3.5 \times 10^{-9}$ |
|                           | $\sigma$  | $\mu$mol cm$^{-2}$ h$^{-1}$ | 0           | 50          |

compared to the data for calibration. There are a total of 21 unknown parameters which correspond to the passive transport processes, the membrane transport processes and the measurement error variance. Uniform priors are used for all parameters. Table 5 shows the parameter units and prior bounds. See Galli and Solidoro (2018) for more detail about the model and the values of the remaining parameters, and Vollert et al (2023) for an application of SMC and analysis of model sloppiness to this model-data calibration problem.

The model is applied to data from Rodolfo-Metalpa et al (2010) measuring the photosynthesis, respiration and calcification of the Mediterranean coral Cladocora caespitosa. The data was measured at winter and summer baseline ($13.4^\circ$C and $21.7^\circ$C) and elevated ($16.4^\circ$C and $24.5^\circ$C) temperatures, two different pCO$_2$ levels (400 and 700 ppm), and under light and dark conditions, giving 16 data points overall.

Figure 13 shows the marginal densities of the three stiffest eigenparameters, figure 14 shows the posterior predictive distribution and table 6 shows the computation cost for SMC and CW-IEKI. Due to the limited data available for this model, the marginal posterior densities for SMC and CW-IEKI are close to the prior (see appendix C). In contrast, the marginal densities of the stiffest eigenparameters shown in figure 13 are much more informative. As with previous examples, the predictive performance of SMC and CW-IEKI are similar, except that the CW-IEKI results have greater uncertainty (figure 14). Again, changing the ESS target threshold for CW-IEKI makes very little difference to the results. For a target threshold of 50%, CW-IEKI is almost 24 times faster than SMC (table 6).
Figure 13. Marginal posterior density plots of the natural logarithm of the three stiffest eigenparameters for the coral model. CW-IEKI results use different ESS target thresholds. Note that the uncertainty parameter $\sigma$ is excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (13). The logarithm of the eigenparameters are calculated based on samples from the prior (black), CW-IEKI (dashed) and SMC (blue) using a sensitivity matrix calculated using the SMC samples.

Figure 14. Comparison of the coral data to the median and 95% central credible intervals for the posterior predictive distribution of coral calcification obtained from the coral model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue).

Table 6. Total and relative number of evaluations of $G(\cdot)$ for SMC and CW-IEKI with different ESS target thresholds for the coral model. Note that the total number of evaluations of $G(\cdot)$ is a multiple of the number of samples $N = 1000$.

| Method | SMC | CW-IEKI |
|--------|-----|---------|
| ESS target threshold | 50% | 95% | 90% | 80% | 70% | 60% | 50% |
| $G(\cdot)$ evaluations | 166 000 | 32 000 | 21 000 | 13 000 | 10 000 | 8 000 | 7 000 |
| Approximate speed-up | 1.00 | 5.19 | 7.90 | 12.77 | 16.60 | 20.75 | 23.71 |

5. Discussion

In this paper, we introduce and test a new method (CW-IEKI) which extends the iterative EKI approach of Iglesias et al (2018) to the case where the covariance matrix has unknown elements.
\( \phi \). CW-IEKI is completely analogous to likelihood tempering SMC, and is a useful alternative to both MCMC and SMC for static Bayesian models of the form \( \mathcal{N}(G(\theta), \Gamma(\phi)) \), where \( \theta \) and \( \phi \) are unknown, and when \( G(\theta) \) is expensive to compute. Note that CW-IEKI can also be applied when the covariance matrix is a function of both \( \theta \) and \( \phi \), as is the case for the six parameter APSIM model applied to the simulated data in section 4.4. That is, CW-IEKI can be applied to models of the form \( \mathcal{N}(G(\theta), \Gamma(\theta, \phi)) \), where \( \theta \mid \phi, y \) is updated using IEKI and \( \phi \mid \theta, y \) is updated using MCMC. Even though the inference from CW-IEKI is biased, we find in practice that it provides reasonable inference even if the likelihood is non-linear Gaussian and the prior is non-Gaussian.

We compare CW-IEKI to SMC on a univariate linear Gaussian example, a population models example and three ecological models applied to real data. On the first two examples, we also compare CW-IEKI to IEKI, and find that CW-IEKI consistently outperforms the latter when the covariance is misspecified. In the linear Gaussian model, the population models example, the three parameter APSIM model and the coral model, the accuracy of CW-IEKI and SMC are similar, but for the remaining models there is clear bias in the marginal posteriors for some of the parameters. Based on the stiffest eigenparameters however, the model parameters showing the most bias also has little impact on the model fit. We find that CW-IEKI has relatively similar predictive performance to SMC—except that the uncertainty of the predictions is consistently overestimated—but advantageously requires around 30 times fewer evaluations of \( G(\cdot) \) on average.

In all of the examples the point predictions from our novel CW-IEKI method are quite accurate, but the uncertainty intervals are inflated relative to SMC, especially when the number of parameters is increased. We find that predictions can be improved by first obtaining \( \phi \) samples from a single run of CW-IEKI, then running CW-IEKI a second time with \( \phi \) fixed at the samples from the initial run. We refer to this approach as two-stage CW-IEKI, and give results in the appendices. An advantage of two-stage CW-IEKI is that it requires an initial run of CW-IEKI, meaning that CW-IEKI can be run, and if computation resources are still available, the second stage can then be applied. In this way, it can be seen as a post-processing method.

If exact inferences are desired, CW-IEKI proposals could potentially be used to speed up exact SMC, for example by incorporating them in the delayed-acceptance SMC algorithm of Bon et al (2021). The inferences from CW-IEKI could also potentially be improved by following the approach of Lan et al (2022) to build an emulator \( \tilde{G}(\cdot) \) of \( G(\cdot) \) using all evaluations of \( G(\cdot) \) from CW-IEKI. An MCMC or SMC algorithm can then be used to target the approximate posterior distribution based on this emulator, i.e. \( \mathcal{N}(y \mid \tilde{G}(\theta), \Gamma(\phi))p(\theta, \phi) \).

An area of future work is to improve the updates in CW-IEKI for the noise parameters \( \phi \). Currently, a fixed number of random-walk MCMC iterations are used. Adapting the number of MCMC iterations and using more efficient updates for \( \phi \), such as the Metropolis-adjusted Langevin algorithm (Girolami and Calderhead 2011) or Hamiltonian Monte Carlo (Betancourt 2017), may improve the performance of the method, especially if \( \phi \) is high-dimensional or its elements are highly correlated. Another extension is to apply the CW-IEKI method to the hierarchical setting explored in Chada et al (2018).

It would be interesting to see whether our approach can be incorporated into the ensemble Kalman sampler of Garbuno-Inigo et al (2020), or the EKI method of Duffield and Singh (2022) for general likelihoods. In the latter case, it may be possible to update some of the model parameters with EKI and some with MCMC, depending on the form of the likelihood function. The potential advantage of such a hybrid approach is that it may significantly improve the accuracy of the final samples, given that the MCMC update targets the exact conditional posterior, while the EKI portion targets some approximation to the conditional posterior.
It would also be interesting to incorporate ideas from CW-IEKI into the method of Wu et al (2022), which uses EKI as the forward kernel in data annealing SMC. This approach is exact, and requires much fewer evaluations of $G(\cdot)$ than SMC with a Metropolis–Hastings forward kernel, but it currently requires the covariance of the likelihood function to be known. One extension here is developing a likelihood tempering SMC algorithm with our CW-IEKI method as the forward kernel. It may also be possible to extend their SMC algorithm to general likelihood models, such that a subset of the parameters are updated using the method of Duffield and Singh (2022), and the rest are updated using an MCMC forward kernel.

Data availability statement

The data cannot be made publicly available upon publication because they are owned by a third party and the terms of use prevent public distribution. The data that support the findings of this study are available upon reasonable request from the authors. MATLAB code for the examples in sections 4.2 and 4.3 is available at https://github.com/imkebotha/cwieki (Botha 2023).

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Appendix A. Extra results for the APSIM model

A.1. Three parameter APSIM model applied to the real data

Figure 15. Marginal posterior density plots for the three parameter APSIM model applied to the real data. Results shown are for two-stage CW-IEKI.

Figure 16. Marginal posterior density plots of the natural logarithm of the eigenparameters for the three parameter APSIM model applied to the real data. Note that the uncertainty parameter $\sigma$ is excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (13). The logarithm of the eigenparameters are calculated based on samples from the prior (black), CW-IEKI (dashed red-orange) and SMC (blue) using a sensitivity matrix calculated using the SMC samples. Results shown are for two-stage CW-IEKI.
Figure 17. Comparison of the real data to the median and 95% central credible intervals for the posterior predictive distribution of cumulative nitrogen mineralisation obtained from the three parameter APSIM model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). Results shown are for two-stage CW-IEKI.

A.2. Six parameter APSIM model applied to the real data

Figure 18. Marginal posterior density plots for the six parameter APSIM model applied to the real data. Results shown are for two-stage CW-IEKI.
Figure 19. Marginal posterior density plots of the natural logarithm of the three stiffest eigenparameters for the six parameter APSIM model applied to the real data. Note that the uncertainty parameter $\sigma$ is excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (13). The logarithm of the eigenparameters are calculated based on samples from the prior (black), CW-IKEI (dashed red-orange) and SMC (blue) using a sensitivity matrix calculated using the SMC samples. Results shown are for two-stage CW-IKEI.

Figure 20. Comparison of the real data to the median and 95% central credible intervals for the posterior predictive distribution of cumulative nitrogen mineralisation obtained from the six parameter APSIM model fitted to this data. Models were fitted using CW-IKEI (red-orange) and likelihood tempering SMC (blue). Results shown are for two-stage CW-IKEI.
A.3. Six parameter APSIM model applied to the simulated data

Figure 21. Marginal posterior density plots for the six parameter APSIM model applied to the simulated data. Results shown are for two-stage CW-IEKI.

Figure 22. Marginal posterior density plots of the natural logarithm of the three stiffest eigenparameters for the six parameter APSIM model applied to the simulated data. Note that the uncertainty parameter $\sigma$ is excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (13). The logarithm of the eigenparameters are calculated based on samples from the prior (black), CW-IEKI (dashed red-orange) and SMC (blue) using a sensitivity matrix calculated using the SMC samples. Results shown are for two-stage CW-IEKI.
Figure 23. Comparison of the simulated data to the median and 95% central credible intervals for the posterior predictive distribution of cumulative nitrogen mineralisation obtained from the six parameter APSIM model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). Results shown are for two-stage CW-IEKI.
Appendix B. Extra results for the seagrass model

Figure 24. Marginal posterior density plots for the seagrass model applied to the *C. serrulata* data. Results shown are for two-stage CW-IEKI.
Figure 25. Marginal density plots of the six stiffest eigenparameters (calculated using equation (15)) for the seagrass model applied to the *C. serrulata* data. Note that the uncertainty parameters in $\phi$ are excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (15). The eigenparameters are calculated based on samples from the prior (black), CW-IEKI (dashed) and SMC (blue) using a sensitivity matrix calculated using the SMC samples. Results shown are for two-stage CW-IEKI.

Figure 26. Comparison of the *C. serrulata* data to the median and 95% central credible intervals for the posterior predictive distribution of net carbon fixation obtained from the seagrass model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). P-I = photosynthesis-irradiance and PAR = photosynthetically active radiation (see Adams *et al* 2020). Results shown are for two-stage CW-IEKI.
Figure 27. Comparison of the *C. serrulata* data to the median and 95% central credible intervals for the posterior predictive distribution of shoot density obtained from the seagrass model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). SI = surface irradiance and 'hot' or 'cold' indicates the temperature conditions under which the seagrass data was collected (Adams et al 2020). Results shown are for two-stage CW-IEKI.

Table 7. Total and relative number of evaluations of $G(\cdot)$ for SMC and CW-IEKI with different ESS target thresholds. Results are for the seagrass model applied to the *C. serrulata* data. Note that the total number of evaluations of $G(\cdot)$ is a multiple of the number of samples $N = 1000$. Results shown are for two-stage CW-IEKI.

| Method  | SMC | CW-IEKI |
|---------|-----|---------|
| ESS target threshold | 50% | 95% | 90% | 80% | 70% | 60% | 50% |
| $G(\cdot)$ evaluations | 799 000 | 87 000 | 60 000 | 39 000 | 30 000 | 24 000 | 20 000 |
| Approximate speed-up | 1.00 | 9.18 | 13.32 | 20.49 | 26.63 | 33.29 | 39.95 |
Figure 28. Marginal posterior density plots for the seagrass model applied to the *H. uninervis* data.
Figure 29. Marginal posterior density plots for the seagrass model applied to the *H. uninervis* data. Results shown are for two-stage CW-IEKI.
Figure 30. Marginal density plots of the six stiffest eigenparameters (calculated using equation (15)) for the seagrass model applied to the *H. uninervis* data. Note that the uncertainty parameters in $\phi$ are excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (15). The eigenparameters are calculated based on samples from the prior (black), CW-IEKI (dashed) and SMC (blue) using a sensitivity matrix calculated using the SMC samples.

Figure 31. Marginal density plots of the six stiffest eigenparameters (calculated using equation (15)) for the seagrass model applied to the *H. uninervis* data. Note that the uncertainty parameters in $\phi$ are excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (15). The eigenparameters are calculated based on samples from the prior (black), CW-IEKI (dashed) and SMC (blue) using a sensitivity matrix calculated using the SMC samples. Results shown are for two-stage CW-IEKI.
Figure 32. Eigenvectors of the six stiffest eigenparameters for the seagrass model applied to the *H. uninervis* data. These results are based on the SMC posterior samples. The labels on the left-hand side correspond to $v_k(\lambda_k/\lambda_1)$, where $v_k$ and $\lambda_k$ are the eigenvector and associated eigenvalue of eigenparameter $k$, respectively. The shade of the cells in row $k$ indicate the relative contribution ($v_k$) of the $j$th parameter to eigenparameter $k$—parameters with darker colours have the greatest contribution.

Figure 33. Comparison of the *H. uninervis* data to the median and 95% central credible intervals for the posterior predictive distribution of net carbon fixation obtained from the seagrass model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). P-I = photosynthesis-irradiance and PAR = photosynthetically active radiation (see Adams *et al* 2020).
Figure 34. Comparison of the *H. uninervis* data to the median and 95\% central credible intervals for the posterior predictive distribution of net carbon fixation obtained from the seagrass model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). P-I = photosynthesis-irradiance and PAR = photosynthetically active radiation (see Adams et al 2020). Results shown are for two-stage CW-IEKI.

Figure 35. Comparison of the *H. uninervis* data to the median and 95\% central credible intervals for the posterior predictive distribution of shoot density obtained from the seagrass model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). SI = surface irradiance and ‘hot’ or ‘cold’ indicates the temperature conditions under which the seagrass data was collected (Adams et al 2020).
Figure 36. Comparison of the *H. uninervis* data to the median and 95% central credible intervals for the posterior predictive distribution of shoot density obtained from the seagrass model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). SI = surface irradiance and ‘hot’ or ‘cold’ indicates the temperature conditions under which the seagrass data was collected (Adams et al 2020). Results shown are for two-stage CW-IEKI.

Table 8. Total and relative number of evaluations of $G(\cdot)$ for SMC and CW-IEKI with different ESS target thresholds. Results are for the seagrass model applied to the *H. uninervis* data. Note that the total number of evaluations of $G(\cdot)$ is a multiple of the number of samples $N = 1000$.

| Method | SMC | CW-IEKI |
|--------|-----|---------|
| ESS target threshold | 50% | 95% | 90% | 80% | 70% | 60% | 50% |
| $G(\cdot)$ evaluations | 594 000 | 87 000 | 58 000 | 38 000 | 29 000 | 24 000 | 20 000 |
| Approximate speed-up | 1.00 | 6.83 | 10.24 | 15.63 | 20.48 | 24.75 | 29.70 |
Table 9. Total and relative number of evaluations of $G(\cdot)$ for SMC and CW-IEKI with different ESS target thresholds. Results are for the seagrass model applied to the *H. uninervis* data. Note that the total number of evaluations of $G(\cdot)$ is a multiple of the number of samples $N = 1000$. Results shown are for two-stage CW-IEKI.

| Method | SMC | two-stage CW-IEKI |
|--------|-----|-------------------|
| ESS target threshold | 50% | 95% | 90% | 80% | 70% | 60% | 50% |
| $G(\cdot)$ evaluations | 594 000 | 156 000 | 106 000 | 68 000 | 52 000 | 43 000 | 36 000 |
| Approximate speed-up | 1.00 | 3.81 | 5.60 | 8.74 | 11.42 | 13.81 | 16.50 |

Figure 37. Marginal posterior density plots for the seagrass model applied to the *Z. muelleri* data.
Figure 38. Marginal posterior density plots for the seagrass model applied to the *Z. muelleri* data. Results shown are for two-stage CW-IEKI.
Figure 39. Marginal density plots of the six stiffest eigenparameters (calculated using equation (15)) for the seagrass model applied to the *Z. muelleri* data. Note that the uncertainty parameters in $\phi$ are excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (15). The eigenparameters are calculated based on samples from the prior (black), CW-IEKI (dashed) and SMC (blue) using a sensitivity matrix calculated using the SMC samples.

Figure 40. Marginal density plots of the six stiffest eigenparameters (calculated using equation (15)) for the seagrass model applied to the *Z. muelleri* data. Note that the uncertainty parameters in $\phi$ are excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (15). The eigenparameters are calculated based on samples from the prior (black), CW-IEKI (dashed) and SMC (blue) using a sensitivity matrix calculated using the SMC samples. Results shown are for two-stage CW-IEKI.
Figure 41. Eigenvectors of the six stiffest eigenparameters for the seagrass model applied to the *Z. muelleri* data. These results are based on the SMC posterior samples. The labels on the left-hand side correspond to $v_k(\lambda_k/\lambda_1)$, where $v_k$ and $\lambda_k$ are the eigenvector and associated eigenvalue of eigenparameter $k$, respectively. The shade of the cells in row $k$ indicate the relative contribution ($v_k$) of the $j$th parameter to eigenparameter $k$ — parameters with darker colours have the greatest contribution.

Figure 42. Comparison of the *Z. muelleri* data to the median and 95% central credible intervals for the posterior predictive distribution of net carbon fixation obtained from the seagrass model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). P-I = photosynthesis-irradiance and PAR = photosynthetically active radiation (see Adams et al 2020)
Figure 43. Comparison of the *Z. muelleri* data to the median and 95% central credible intervals for the posterior predictive distribution of net carbon fixation obtained from the seagrass model fitted to this data. Models were fitted using CW-IIEKI (red-orange) and likelihood tempering SMC (blue). P-I = photosynthesis-irradiance and PAR = photosynthetically active radiation (see Adams et al 2020). Results shown are for two-stage CW-IIEKI.

Figure 44. Comparison of the *Z. muelleri* data to the median and 95% central credible intervals for the posterior predictive distribution of shoot density obtained from the seagrass model fitted to this data. Models were fitted using CW-IIEKI (red-orange) and likelihood tempering SMC (blue). SI = surface irradiance and ‘hot’ or ‘cold’ indicates the temperature conditions under which the seagrass data was collected (Adams et al 2020).
Figure 45. Comparison of the *Z. muelleri* data to the median and 95% central credible intervals for the posterior predictive distribution of shoot density obtained from the seagrass model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). SI = surface irradiance and ‘hot’ or ‘cold’ indicates the temperature conditions under which the seagrass data was collected (Adams *et al* 2020). Results shown are for two-stage CW-IEKI.
Table 10. Total and relative number of evaluations of $G(\cdot)$ for SMC and CW-IEKI with different ESS target thresholds. Results are for the seagrass model applied to the Z. *muelleri* data. Note that the total number of evaluations of $G(\cdot)$ is a multiple of the number of samples $N = 1000$. 

| Method         | SMC      | CW-IEKI  |
|----------------|----------|----------|
| ESS target threshold | 50%     | 95% 90% 80% 70% 60% 50% |
| $G(\cdot)$ evaluations | 686 000 | 68 000 66 000 30 000 23 000 19 000 16 000 |
| Approximate speed-up | 1.00    | 10.09 14.91 22.87 22.87 22.87 |

Table 11. Total and relative number of evaluations of $G(\cdot)$ for SMC and CW-IEKI with different ESS target thresholds. Results are for the seagrass model applied to the Z. *muelleri* data. Note that the total number of evaluations of $G(\cdot)$ is a multiple of the number of samples $N = 1000$. **Results shown are for two-stage CW-IEKI.**

| Method             | SMC      | two-stage CW-IEKI |
|--------------------|----------|-------------------|
| ESS target threshold | 50% | 95% 90% 80% 70% 60% 50% |
| $G(\cdot)$ evaluations | 686 000 | 126 000 85 000 56 000 43 000 35 000 30 000 |
| Approximate speed-up | 1.00   | 5.44 8.07 12.25 15.95 19.60 22.87 |
Appendix C. Extra results for the coral model

Figure 46. Marginal posterior density plots for the coral model
Figure 47. Marginal posterior density plots for the coral model. Results shown are for two-stage CW-IEKI.
Figure 48. Marginal posterior density plots of the natural logarithm of the three stiffest eigenparameters for the coral model. CW-IEKI results use different ESS target thresholds. Note that the uncertainty parameter $\sigma$ is excluded from the analysis of sloppiness, and $\lambda_k$ is the eigenvalue associated with eigenvector $v_k$ in equation (13). The logarithm of the eigenparameters are calculated based on samples from the prior (black), CW-IEKI (dashed) and SMC (blue) using a sensitivity matrix calculated using the SMC samples. Results shown are for two-stage CW-IEKI.

Figure 49. Comparison of the coral data to the median and 95% central credible intervals for the posterior predictive distribution of coral calcification obtained from the coral model fitted to this data. Models were fitted using CW-IEKI (red-orange) and likelihood tempering SMC (blue). Results shown are for two-stage CW-IEKI.
Table 12. Total and relative number of evaluations of $G(\cdot)$ for SMC and CW-IEKI with different ESS target thresholds for the coral model. Note that the total number of evaluations of $G(\cdot)$ is a multiple of the number of samples $N = 1000$. Results shown are for two-stage CW-IEKI.

| Method  | SMC | CW-IEKI |
|---------|-----|---------|
| ESS target threshold | 50% | 95% | 90% | 80% | 70% | 60% | 50% |
| $G(\cdot)$ evaluations | 166 000 | 61 000 | 42 000 | 27 000 | 20 000 | 16 000 | 14 000 |
| Approximate speed-up | 1.00 | 2.72 | 3.95 | 6.15 | 8.30 | 10.38 | 11.86 |

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