Supplementary Material

"Quantifying parameter-induced uncertainty and evaluating the effects of model simplification in a marine biogeochemical model"

S1 Updates to the Eco3M-MED-V1b model

Eco3M-MED-V1b includes only minor revisions relative to the Eco3M-MED-V1a used in our previous study (Zhang et al., 2026). The main modification concerns nutrient uptake: the inhibition terms included in the previous configuration were removed. No major changes were made to the ecosystem structure. Eco3M-MED-V1b is a version very close to Eco3M-MED-V2. A detailed description of Eco3M-MED-V2 (which is also applicable to Eco3M-MED-V1b), including its updated parameterisation approach, is provided in Baklouti et al. (under review).

S2 Comparison between reference simulation and ensemble median

Figure S1 compares the reference simulation $\hat{m}$ with the ensemble median $\widetilde{m}$ for the FULL model, and shows their difference throughout the water column.

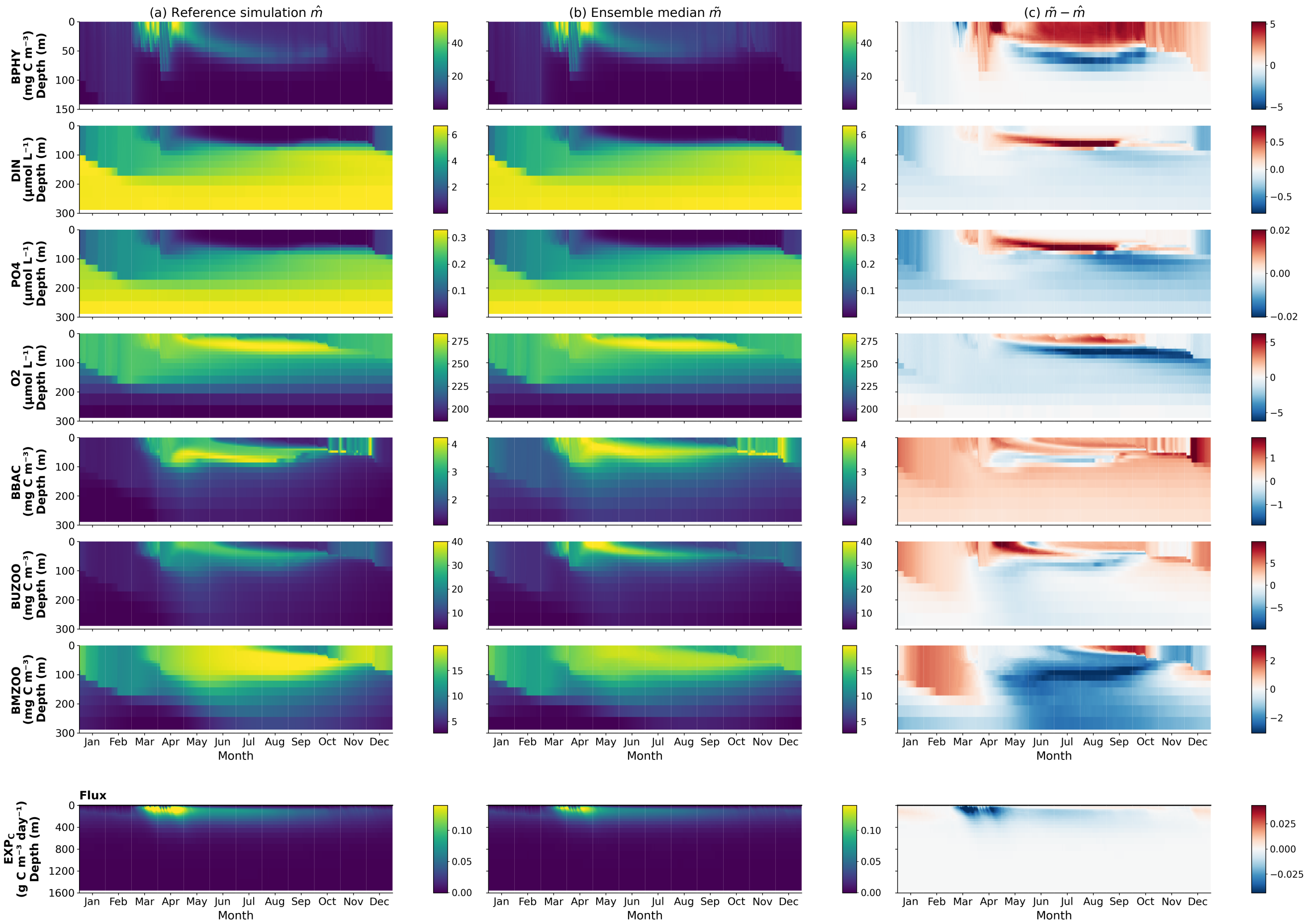

Figure S1: Comparison between the reference simulation and the ensemble median for the FULL model. Panel (a) shows the reference simulation $\hat{m}$, Panel (b) shows the ensemble median $\widetilde{m}$, and Panel (c) shows the difference between the median and reference value (i.e. $\widetilde{m} - \hat{m}$).

S3 Sobol ensemble generation and convergence diagnostics

To determine whether the ensemble size was sufficient, the ensemble statistics were recalculated using the first $N = 16, 32, 64, 128, 256, 512$ members of the same Sobol sequence. Each larger subset therefore contained all members of the preceding smaller subset. For each ecosystem indicator and model versions, we calculated the ensemble median $\widetilde{m}_N$ and the uncertainty spread Δ_N. Their stability was then evaluated between successive ensemble sizes by comparing the estimates obtained with N members with those obtained with $N/2$ members.

The relative change in the ensemble median was defined as:

$$C_N(\tilde{m}) = \frac{|\tilde{m}_N - \tilde{m}_{N/2}|}{\Delta_{512}} \times 100\% \tag{S1}$$

and the relative change in the uncertainty spread as:

$$C_N(\Delta) = \frac{|\Delta_N - \Delta_{N/2}|}{\Delta_{512}} \times 100\% \tag{S2}$$

Fig. S2 shows that changes in the ensemble median were already small after the first few ensemble doubling steps, whereas the spread required larger ensemble sizes to stabilise.

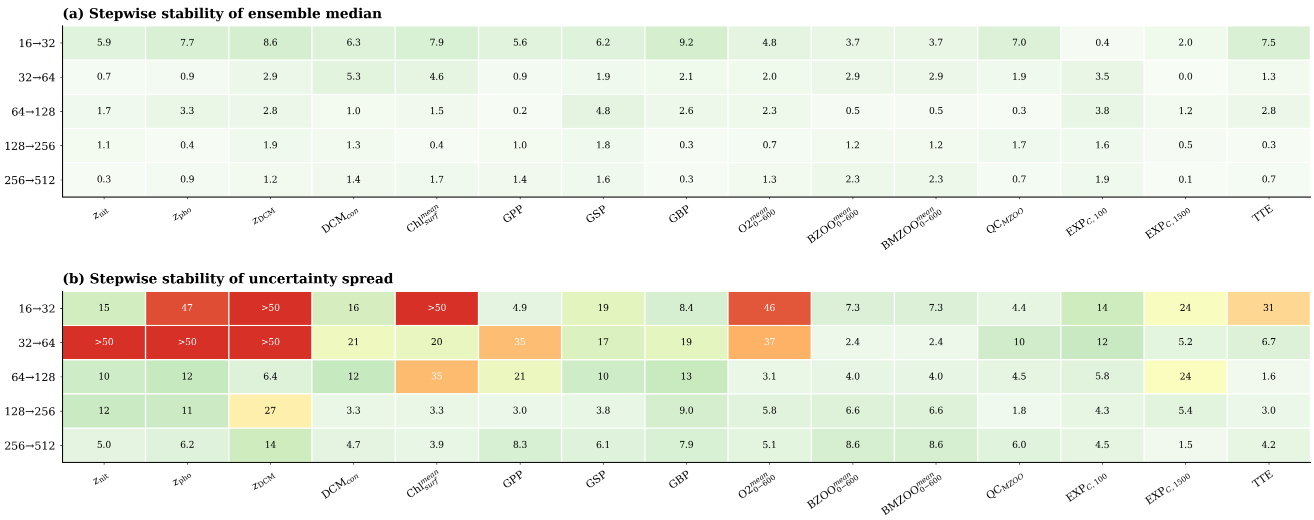

Figure S2: Stepwise convergence of the ensemble statistics for the ecosystem indicators. Panel (a) shows the ensemble median change, and panel (b) shows the uncertainty spread change when the ensemble size increased from $N/2$ to N. For each indicator and ensemble size, the plotted value is the largest change obtained among FULL, MOD1, and MOD2. Changes are expressed by $C_N(\tilde{m})$ and $C_N(\Delta)$.

At the final doubling step ($N = 256 \rightarrow 512$), the ensemble medians were relative stable for all ecosystem indicators in all three model versions, with a maximum change of 2.35%. The uncertainty spread was also generally stable.

Figure S3 provides an additional assessment of ensemble convergence for the FULL version. For each ecosystem indicator, the median and the 5th–95th percentile range were calculated using increasing ensemble sizes. Between $N = 256$ and $N = 512$, the median changed only slightly for most indicators, indicating that the main distribution statistics were relatively stable with 512 ensemble members.

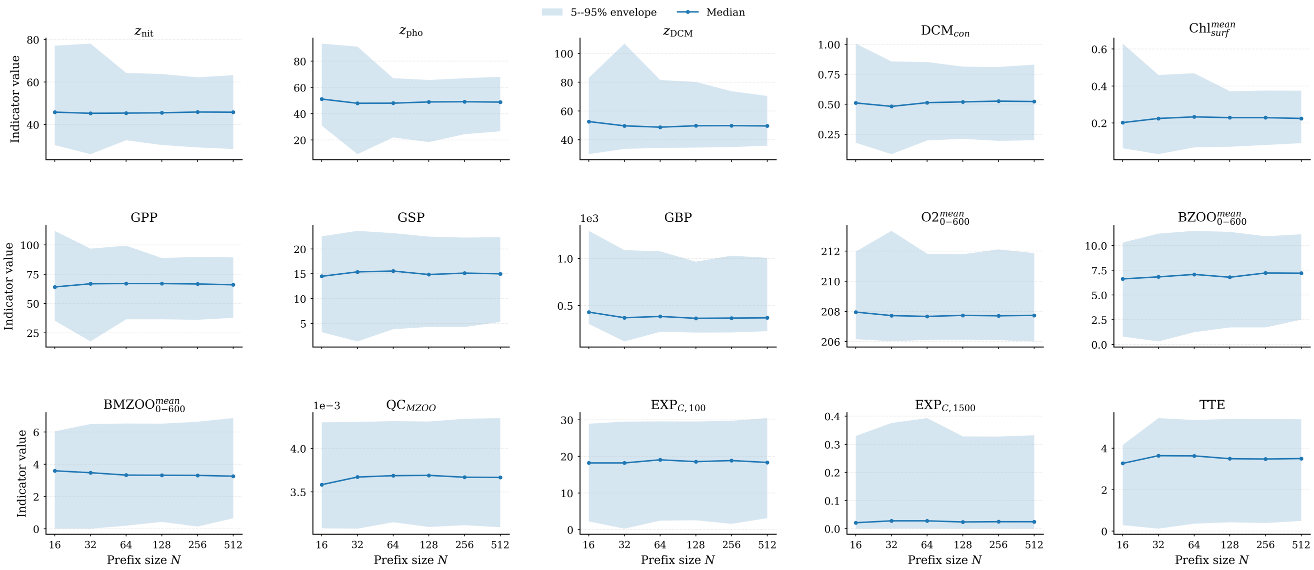

Figure S3: Evolution of ecosystem indicator distributions as the sample size increases (case for FULL version). The shaded area denotes the 5th–95th percentile envelope, and the solid line denotes the ensemble median. Values are in the original units of each indicator (not shown here).

S4 One-to-one ensemble member comparison

The one-to-one comparison helps interpret the lower-tail and extreme responses (Fig. S4). For several biological and carbon export indicators, including DCM_{con}, GBP, BZOO, BMZOO, $\mathrm{EXP}_{C,100}$, and $\mathrm{EXP}_{C,1500}$, parameter sets that produce low values in FULL generally also produce low values in MOD1 and MOD2. Similarly, parameter sets producing high values in FULL often remain associated with high values in the simplified versions. This one-to-one comparison indicates that the lower-tail and extreme responses are largely linked to particular parameter combinations, rather than due to the model simplification directly.

S5 Choice of 90% ensemble range as uncertainty spread

Fig. S5 shows that most ensemble members are concentrated within the central part of each indicator distribution, while a limited number of members were found outside the 5th–95th percentile range. Several indicators including GPP, GSP, BZOO, BMZOO, and $\mathrm{EXP}_{C,1500}$, show lower-tail values close to zero, whereas some indicators also show isolated high values.

Therefore, the full minimum–maximum range of ensemble is highly sensitive to a small number of extreme ensemble members and may provide an unstable estimate of uncertainty. For this reason, the uncertainty spread used in this study was defined as the central 90% ensemble range, $\Delta = q_{0.95} - q_{0.05}$, as commonly used by other similar studies with the same objective (Murphy et al., 2004; Smith et al., 2009) .

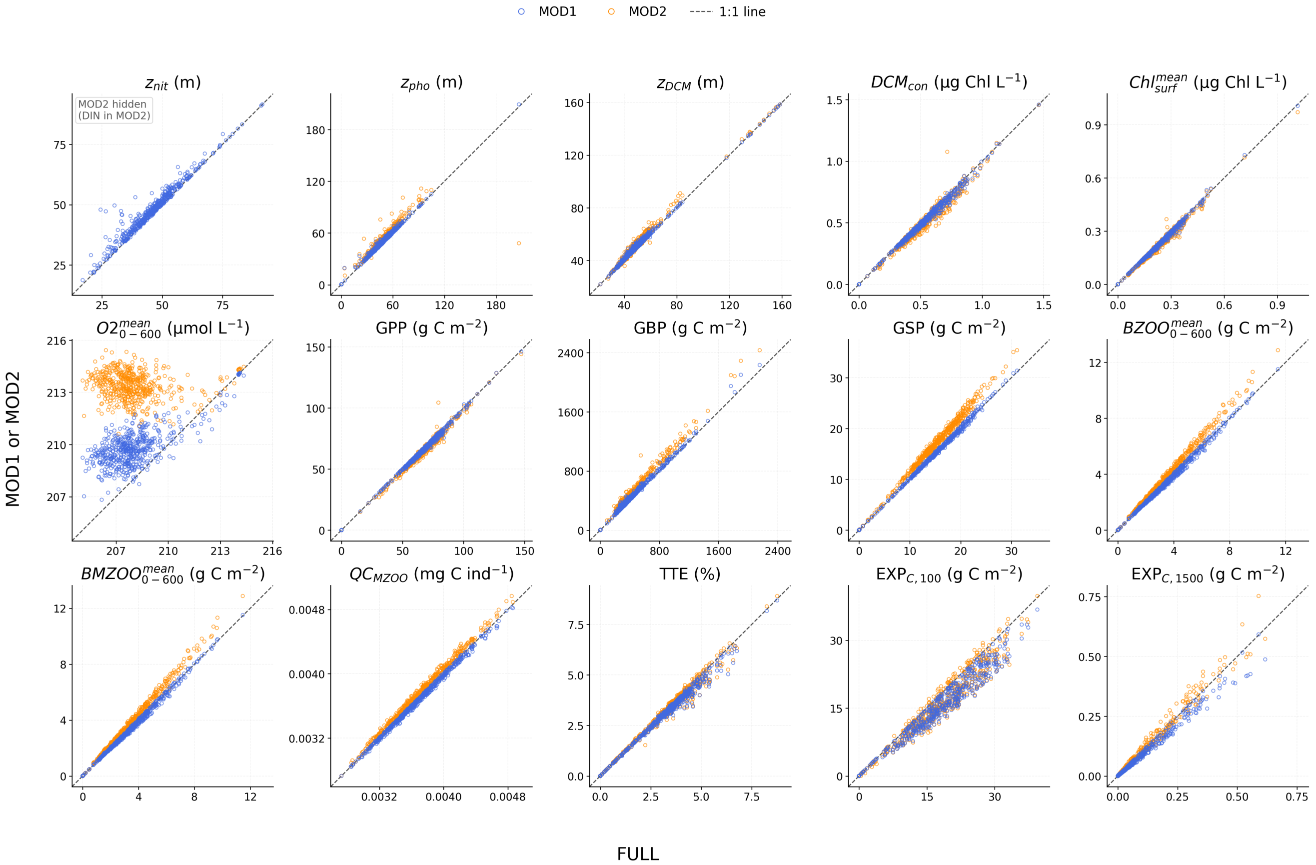

Figure S4: One-to-one comparisons of ecosystem indicators among MOD1, MOD2 and FULL. Blue points denote MOD1, orange points denote MOD2, and the dashed grey line indicates the 1:1 reference relative to FULL. z_{nit} is not presented in MOD2.

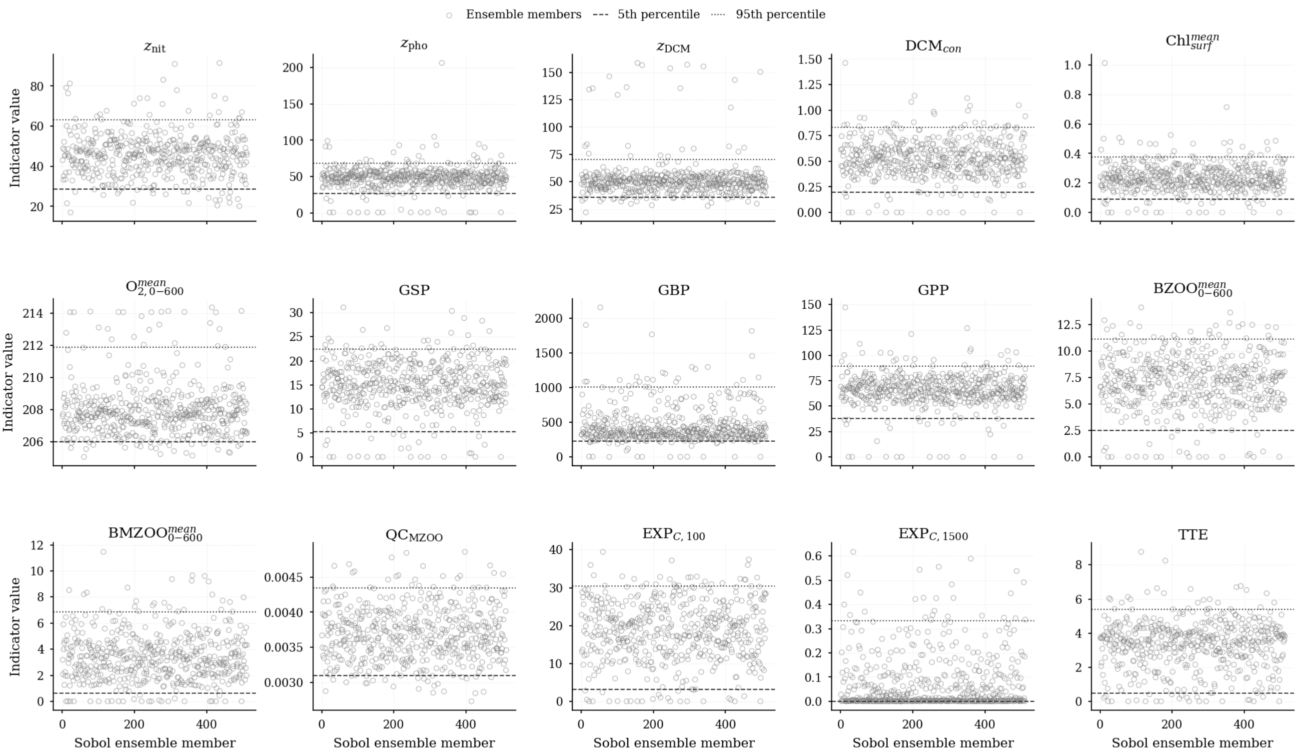

Figure S5: Relationships among production, trophic, and export-related indicators in the FULL ensemble simulations. Each panel shows one indicator, and each point corresponds to one ensemble member. Dashed and dotted horizontal lines indicate the 5th and 95th percentiles, respectively.

S6 Seasonal vertical profiles of microbial food web

To further examine the microbial food web, Fig. S6 compares the seasonal vertical profiles of bacterial and zooplankton biomass (BHNF, BCIL and BMZOO) among the three model versions. We can see that MOD2 generally shows higher bacterial and zooplankton biomass, and extending to deeper depths.

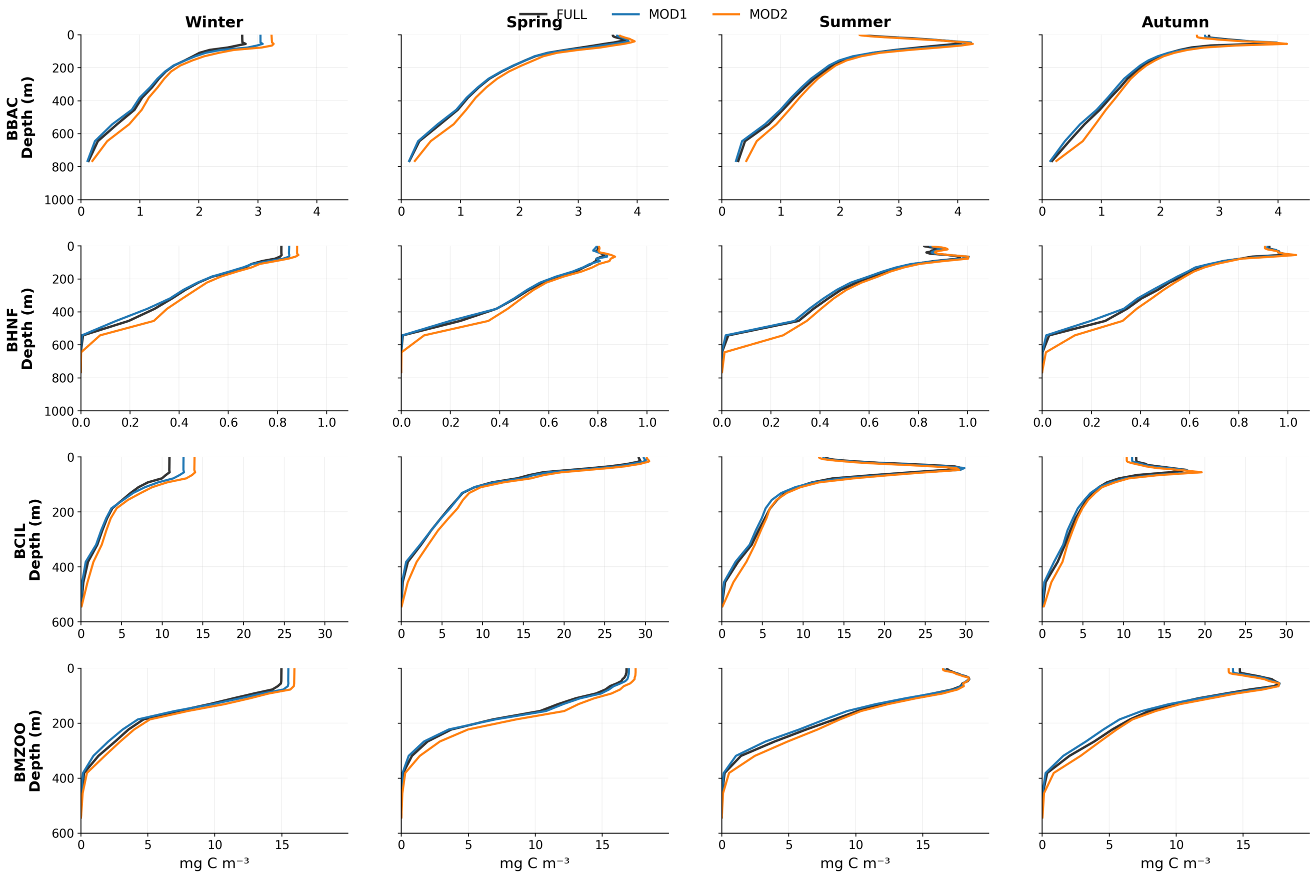

Figure S6: Seasonal vertical profiles of ensemble median BBAC, BHNF, BCIL, and BMZOO in FULL (black line), MOD1 (blue line), and MOD2 (red line).

References

Baklouti, M., Zhang, Y., Mazoyer, C., Barrier, N., Pagès, R., under review. A new method for consistent and simplified parameterization of marine biogeochemical models: Application to the Eco3M-MED V2 model in the mediterranean sea Manuscript submitted to Journal of Advances in Modeling Earth Systems.

Murphy, J.M., Sexton, D.M., Barnett, D.N., Jones, G.S., Webb, M.J., Collins, M., Stainforth, D.A., 2004. Quantification of modelling uncertainties in a large ensemble of climate change simulations. Nature 430, 768–772. doi:https://doi.org/10.1038/nature02771.

Smith, R.L., Tebaldi, C., Nychka, D., Mearns, L.O., 2009. Bayesian modeling of uncertainty in ensembles of climate models. Journal of the American Statistical Association 104, 97–116. doi:10.1198/jasa.2009.0007.

Zhang, Y., Baklouti, M., Brasseur, P., Debreu, L., 2026. A semi-automated sensitivity-based approach for simplifying marine biogeochemical models for targeted applications: A case study with the eco3m-med model. Ecological Modelling 514, 111491. doi:https://doi.org/10.1016/j.ecolmodel.2026.111491.