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SPUX: A new flexible method for uncertainty quantification with particle Markov Chain Monte Carlo - An application to aquatic ecology

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In recent years, theoretical advancements and the steady increase in computational power have allowed mathematical models to reduce their level of approximation to reality by increasing complexity and/or by achieving better convergence.

However, complex computational models require scalability, expensive calibration campaigns, and comparative assessments of the results. The last two goals constitute the core of Uncertainty Quantification (UQ) techniques. However, the application of UQ methods has been hindered by the complex nature of the underlying models, and by the general slow convergence of Monte Carlo methods, which is often exacerbated when dealing with stochastic models.

Here we present a general Python framework named SPUX that uses particle filtering coupled with, possibly interacting, parallel Markov Chain Monte Carlo (MCMC) runs. The evaluation of the likelihood function for a given set of parameters values is performed by propagating an ensemble of model simulations (particles) at each step of each MCMC in parallel. At each available observational time, the likelihood of each particle is evaluated, and particles are killed and cloned (re-sampled) accordingly. When the latest observational time is reached, a consensus likelihood is computed by gathering all the collected information from each particle, and the gauged parameters values are either accepted or rejected. By applying this framework to a multi-species individual-based model that describes the evolution of an aquatic invertebrate community given multiple observations from independent experiments with different levels of contaminants, we show that we are able to achieve faster parameter convergence and higher accuracy by mitigating the effect of the stochastic model propagation, and by using parallel computing resources fully.