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Uncertainty quantification for massive autonomous systems based on a second-order adjoint method

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Data assimilation (DA) is a fundamental computational technique that integrates numerical simulation models and observation data based on Bayesian statistics. One key issue is the implementation of DA in massive simulation models under the constraints of computational time and resources. We propose a new adjoint-based DA methodology based on the four-dimensional variation method (4DVar) implemented a second-order adjoint method, which produces not only optimum estimates but also their uncertainties within the reasonable computational limitations. The uncertainties are given as diagonal elements of the inverse of Hessian matrix, which is the covariance matrix of a Gaussian that approximates the posterior distribution in the neighborhood of the optimum. Conventional algorithms for deriving the Hessian inverse require $O(CN^2 + N^3)$ computations and $O(N^2)$ memory, where N is the degree of freedom of a given autonomous system and C is the number of computations needed to simulate time series of suitable time length. The proposed method using a second-order adjoint method allows us to directly evaluate the diagonal elements of the Hessian inverse without computing all of its elements. This drastically reduces the number of computations to $O(C)$ and the amount of memory to $O(N)$ for each diagonal element. The proposed method is validated through numerical tests using a massive two-dimensional Kobayashi phase-field model. We confirm that the proposed method correctly reproduces the parameter and initial state assumed in advance, and successfully evaluates the uncertainty of the parameter.