A posteriori goal ensembles

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Current models of Geophysical Fluid Dynamics (GFD) lack the capability to quantify computationally induced errors. To address this issue, we present a new approach for numerical uncertainty quantification in GFD models: a posteriori goal ensembles. We estimate the error in selected physical quantities -- so-called goals -- as a weighted sum of local model errors. Our algorithm divides this goal error estimation into three phases. In phase one, we describe local model errors as a local stochastic process. In phase two, a learning algorithm adapts the selected stochastic process to a given numerical experiment by determining its free parameters, e.g., mean and variance. To do this, the learning algorithm analyzes a series of short numerical simulations on different resolutions. In phase three, different realizations of the local stochastic process produce a goal error estimate ensemble that can be used to construct error bounds for the original goal approximation. The required weights for the weighted sum of local model errors are the sensitivities of the goal with respect to local model errors. These sensitivities are calculated automatically with an Algorithmic Differentiation tool applied to the model's source code. We evaluate the algorithm within a numerical model for the shallow water equations on the sphere, and implement an Algorithmic Differentiation framework that calculates any required goal sensitivity. The description of numerical local errors as a stochastic process allows us to estimate an ensemble of goal approximation errors from only one forward solution of the model. We compare our posterior ensembles with stochastic physics and initial condition ensembles. For two classical test cases, we see that an a posteriori ensemble that is derived from a single model solution delivers comparable results to a stochastic physics ensemble that requires multiple model solutions. While the testbed of our algorithm is simple compared to modern 3D climate models, it is a complex fluid solver that incorporates many features of a General Circulation Model. The proposed algorithm bridges the gap between deterministic numerical methods and stochastic ensemble methods. It is generally applicable, easy to use, and simple compared to classical goal error estimation methods. We believe that a posteriori ensembles could be a first step towards automatic error bars for GFD models.