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Ensemble-type numerical uncertainty information from single model integrations

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ABSTRACT

We suggest an algorithm that quantifies the discretization error of time-dependent physical quantities of interest (goals) for numerical models of geophysical fluid dynamics. The goal discretization error is estimated using a sum of weighted local discretization errors. The key feature of our algorithm is that these local discretization errors are interpreted as realizations of a random process. The random process is determined by the model and the flow state. From a class of local error random processes we select a suitable specific random process by integrating the model over a short time interval at different resolutions. The weights of the influences of the local discretization errors on the goal are modeled as goal sensitivities, which are calculated via automatic differentiation. The integration of the weighted realizations of local error random processes yields a *posterior ensemble* of goal approximations from a single run of the numerical model. From the posterior ensemble we derive the uncertainty information of the goal discretization error. This algorithm bypasses the requirement of detailed knowledge about the models discretization to generate numerical error estimates. The algorithm is evaluated for the spherical shallow-water equations. For two standard test cases we successfully estimate the error of regional potential energy, track its evolution, and compare it to standard ensemble techniques. The posterior ensemble shares linear-error-growth properties with ensembles of multiple model integrations when comparably perturbed. The posterior ensemble numerical error estimates are of comparable size as those of a stochastic physics ensemble.

1. Introduction

Numerical models of geophysical fluid dynamics (GFD) have inherent and inevitable uncertainties. Numerical uncertainties are usually analyzed during the development phase of the model; the standard approach requires a detailed analysis of the numerical properties of the scheme used. In this paper, we propose an algorithm that allows us to estimate a posteriori the numerical error directly from the model solutions.

The behavior of GFD systems is characterized by physical quantities of interest such as total energy content or transport quantities. These physical quantities can be described as functionals of the model solution and are called “goals”. The algorithm that we propose estimates the error in the calculation of goals due to numerical uncertainties. The starting point of our considerations is the dual-weighted residual method of computational fluid dynamics (e.g., [1,14,5,15,6,2]). In the dual-weighted residual method the estimation of the goal error is split into the estimation of local model errors and the

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sensitivity of the goal to local changes. The sensitivities are calculated as the adjoint solution of a goal-dependent dual problem. In summary, one obtains a (sensitivity-)weighted sum of local errors. In standard forms of the dual-weighted residual methods, the local model errors are estimated using knowledge of the discretization formulation and thus require an in-depth understanding of the underlying discrete model. The latter fact can become prohibitive for complex nonlinear models. So far the quantification of goal approximation errors for GFD applications has been done via deterministic local error estimates [5,16]. Here the local model errors are treated as a uniquely deterministic consequence of the modeled flow, and the goal error is therefore a deterministic consequence of these local errors.

We deviate from the framework of the dual-weighted residual method by treating the local error as a stochastic process. The key element of our approach is the *goal approximation ensemble*. The goal approximation ensemble is calculated in two steps. First, a suitable and specific element of a class of stochastic processes such as the Gaussian processes is selected. The selection uses information from short model integrations at a standard resolution and at a higher resolution to determine the parameters of the stochastic process. Second, from realizations of the selected stochastic process and the adjoint solution a goal approximation ensemble is calculated a posteriori. From this goal approximation ensemble we estimate bounds for the goal error. The calculation of the sensitivity information uses Algorithmic Differentiation [9,13].

The novel aspect of our algorithm is the goal approximation ensemble. This ensemble aims to capture the linear component of information component of a nonlinear model ensemble but generates this information from two short model runs at standard and high resolution, one (forward) integration of the model and one adjoint integration. In terms of computational cost this reduces essentially to a single integration of the model and its adjoint on the lower resolution. We provide numerical evidence that the stochastic characterization of local errors enables us through the goal approximation error to estimate the error in the goal approximation. This work extends our earlier work [16] on deterministic error estimation to a stochastic framework.

This paper is organized as follows: in Section 2 we formulate the general problem: what do we mean when we speak about error bounds for numerical goals? Section 3 presents our proposed algorithm to solve this problem. This section represents the core of our approach and shows where we diverge from classical numerical error estimation techniques. In Section 4 we introduce a model to evaluate our algorithm, and in Section 5 results are shown for this model and two test cases. In Section 6 we discuss the results and especially compare the posterior goal error ensembles with forward ensembles. We conclude in Section 7 with an outlook of potential applications of our algorithm.

2. General problem statement

We keep the problem statement abstract to permit a general formulation of our error estimation algorithm in Section 3. A more specific formulation will be given in Section 4. We introduce a general, continuous model N that maps a state vector $\mathbf{q}$ from its initial value $\mathbf{q}_0$ to its value $\mathbf{q}(t)$ at a later time. The model N might be a linear mapping or a nonlinear one, such as the Shallow-Water Equations in Section 4. The model N acts on the state vector as follows

$$N(\mathbf{q}(\mathbf{x},t)) = 0, \qquad \mathbf{q}(\mathbf{x},t_0) = \mathbf{q}^0(\mathbf{x}), \;\; \mathbf{q}(\mathbf{x},t) = \mathbf{q}_b(t) \qquad \text{on } \partial\Omega, \tag{1}$$

with $\mathbf{q}(\mathbf{x},t)$ the solution state vector on a space (Ω)-time (T) domain $\Omega \times T$, $\mathbf{q}^0$ the initial condition and $\mathbf{q}_b(t)$ the boundary conditions on the boundary $\partial\Omega$. The continuous model N is now discretized in order to calculate a numerical solution. The discrete model N_Δ can be represented in an analogous form

$$N_\Delta(\mathbf{q}_\Delta) = 0, \qquad \mathbf{q}^0_\Delta = P\mathbf{q}^0, \;\; \mathbf{q}_\Delta = P\mathbf{q}_b \qquad \text{on } \partial\Omega_\Delta \tag{2}$$

with $\mathbf{q}_\Delta = (\mathbf{q}^n_\Delta)_n$ the discrete state vector that incorporates all time slices of the state $\mathbf{q}^n_\Delta$ in the discrete space–time domain, and the projection operator P that maps the continuous initial and boundary conditions on the discrete space. We are interested in selected physical quantities $J(\mathbf{q})$ and their discrete approximations $J_\Delta(\mathbf{q}_\Delta)$. The dependency of a goal on the state may include only parts of the full state vector, and it may also only focus on specific regions or times. We are interested in the goal error, defined by

$$\varepsilon_J := J_\Delta(\mathbf{q}_\Delta) - J(\mathbf{q}). \tag{3}$$

As the exact error has a sign and we are looking at stochastic error properties of the model that will create error bounds but not necessarily the correct sign, we define the error bounds as follows. We introduce a posteriori error bounds $\varepsilon_{upper}, \varepsilon_{lower}$, i.e., errors of the goal for a calculated solution $\mathbf{q}_\Delta$. We introduce the upper and lower error bounds that constrain the original functional value

$$\varepsilon_{lower}(\mathbf{q}_\Delta) < J_\Delta(\mathbf{q}_\Delta) - J(\mathbf{q}) < \varepsilon_{upper}(\mathbf{q}_\Delta). \tag{4}$$

We summarize the general problem statement: Given a model N, its discretization N_Δ and specifically its discrete solution ($\mathbf{q}_\Delta$), when looking at a physical quantity J, how can we estimate error bounds ε_{upper} and ε_{lower} that quantify the uncertainty of the goal approximation so that $\varepsilon_J > \varepsilon_{lower}$ and $\varepsilon_J < \varepsilon_{upper}$?