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Stochastic goal-oriented error estimation with memory

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ABSTRACT

We propose a stochastic dual-weighted error estimator for the viscous shallow-water equation with boundaries. For this purpose, previous work on memory-less stochastic dual-weighted error estimation is extended by incorporating memory effects. The memory is introduced by describing the local truncation error as a sum of time-correlated random variables. The random variables itself represent the temporal fluctuations in local truncation errors and are estimated from high-resolution information at near-initial times. The resulting error estimator is evaluated experimentally in two classical ocean-type experiments, the Munk gyre and the flow around an island. In these experiments, the stochastic process is adapted locally to the respective dynamical flow regime. Our stochastic dual-weighted error estimator is shown to provide meaningful error bounds for a range of physically relevant goals. We prove, as well as show numerically, that our approach can be interpreted as a linearized stochastic-physics ensemble.

1. Introduction

Quantifying the uncertainty due to discretization errors is essential in judging the quality of a numerical model solution. For many applications we are not only interested in estimates of the discretization error in certain norms but especially in estimating the resulting error in key physical quantities of interest (goals) such as energetic quantities or volume transports. These goals are linear or non-linear functionals of the model solution. A conceptual framework for this type of error estimation is provided by dual-weighted error estimation techniques [1–7]. Dual-weighted methods are applied to a model solution *a posteriori* and combine the adjoint model solution with residual information; both are deterministic quantities. The adjoint solution is the sensitivity of the goal with respect to the residual. In the context of this study, the residual is the local truncation error that describes to which extend the exact solution to the continuous equations fails to satisfy the discrete equations. A stochastic extension of the dual-weighted error estimation approach was developed in [8] by modeling the local truncation error as a stochastic process. The purpose of this paper is to extend the stochastic dual-weighted error estimation by including memory effects and to gain a more profound theoretical understanding of the properties of stochastic dual-weighted approaches. This is done by theoretical analysis as well as by an experimental evaluation of the new error estimation algorithm.

For practical applications, where continuous model solutions are unavailable, obtaining residual information comes down to two basic approaches [9] that each can be used to drive dual-weighted error estimation. In the first approach, the discrete model solution is inserted into a higher-resolved discrete model which yields what we refer to as the classical

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residual, (see [5]). In the second approach, which is for instance used in [3], a higher-resolved discrete model solution is inserted into the discrete model which yields the local truncation errors.

We propose a stochastic representation of the local truncation error because the established methods for calculating the local truncation error and the classical residual via a higher-order reconstruction are difficult to obtain within our discrete model. The shallow-water model that we use to illustrate our method uses a finite-difference–finite-volume discretization on an unstructured grid with a staggered distribution of variables (Arakawa C-staggering). For such models, a higher-order interpolation of the state vector would for instance require to interpolate the normal components of the velocity vector from an unstructured and non-orthogonal grid at a coarse resolution to the same grid type at higher resolution. This task poses its own difficulties. An additional reason is due to the specific target application for which we aim to develop an error estimation algorithm, namely global ocean modeling. For this model framework, we expect a combination of high computational costs of such a higher-order representation, significant computational costs of the residual evaluation itself, and the typical under-resolution of ocean model solutions, which would make the established methods prohibitive.

An alternative approach to continuously obtaining residual information was introduced in [8] where local truncation errors are modeled as a stochastic process. This approach was proposed and tested for wave-type flows in a shallow-water model. The replacement of deterministic local truncation errors by a stochastic process was motivated by the Mori–Zwanzig formalism [10–13] from statistical mechanics. The Mori–Zwanzig formalism is used here as a conceptual picture that provides us with a guideline of how a model that acts on a limited amount of (finite) scales could be supplemented to incorporate the influence of the unresolved scales. In this, we do not aim for a systematic or rigorous implementation of the Mori–Zwanzig formalism. From the point of view of the resolved scales, the influence of the unresolved scales can then be interpreted as being stochastic. In the dual-weighted error estimation approach, the information about the unresolved dynamics inherently lies within the local truncation errors. Therefore, local truncation errors can be interpreted stochastically as local model uncertainty, and the temporal evolution of this uncertainty can be described by a stochastic process. This poses the question of how to determine a suitable stochastic process. In [8], a white-noise process was chosen, which was in accordance to the flows under consideration. The parameters of the white-noise process were estimated using high-resolution information from short, near-initial time-windows and then extrapolated to longer time periods.

Our work is oriented along the lines of [8], but we go beyond this work in several aspects. First, we extend the algorithm to stochastic processes with memory, a property deemed to be highly important in modeling the effect of the unresolved scales (see e.g. [10–14]). The white-noise process used in [8] does not provide such a memory effect as future states are independent of previous states. Our algorithm now models the local truncation error by considering temporal fluctuations in local truncation errors at all previous timesteps, and thus naturally inherits a memory effect. Second, we deepen the analysis of the algorithm and the algorithm's results, we clarify its relation to ensemble techniques, and we discuss the assumption of the dual-weighted method underlying our approach, namely that the goal discretization error is assumed to be negligible. As a consequence of our algorithmic extension we are able to consider the estimation of errors in goals for two-dimensional flows with boundaries and viscosity.

In the framework of the two-dimensional shallow-water equations, we study two ocean-type experiments, the so-called Munk gyre and the flow around an island. The investigation of viscous flows with lateral boundaries poses several challenges. First, changing the model resolution can now coincide with a change in the model parameters, possibly introducing systematic biases in the local truncation errors that are persistent in time. Thus, local truncation errors at different timesteps cannot be assumed to be uncorrelated. Also, a memory term is needed to account for these biases. Second, we encounter transient flows, such as flows being spun up from initial rest. For these flows, the local truncation errors are expected to grow in time. For these reasons, a white-noise process as it was used in [8] is not sufficient any more. The third issue concerns the presence of lateral boundaries. As the dynamical flow regime near these boundaries changes, so does the production rate of local truncation errors. Information about a change of the flow regime needs to be featured into the stochastic process. We will show how to derive a stochastic process that satisfies these new requirements. An important assumption for our choice of underlying dual-weighted approach, which is for instance derived in [3], is that the error in the goal due to discretization of the goal itself is negligible. Our numerical results indicate that this assumption does not necessarily hold for our experiments. However, we show that, under certain conditions, we can correct for this error and thus still obtain viable error estimates.

The paper is structured as follows: In section 2, we explain the basic dual-weighted error estimation approach for a general framework and connect it to the shallow-water model and our chosen discretized model. Section 3 describes how our specific dual-weighted error estimation framework can be carried into a stochastic framework. Based on this stochastic framework, we propose an algorithm to goal-oriented error estimation in Section 4. Section 5 describes the results of our error estimation algorithm on the two experiments including a discussion of the results, and in section 6 we conclude.

2. The shallow-water equations and goal errors

The model that we use to illustrate our stochastic error estimation approach are the viscous shallow-water equations on the sphere, which are here given in the vector-invariant form by