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A Fast and Robust Optimization Methodology for a Marine Ecosystem Model Using Surrogates

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Abstract

Model calibration in climate science plays a key role for simulations and predictions of the earth's climate system. Straightforward attempts by employing the high-fidelity (or fine) model under consideration directly in an optimization loop using conventional optimization algorithms are often tedious or even infeasible, since typically a large number of computationally expensive fine model evaluations are required. The development of faster methods becomes critical, where the optimization of coupled marine ecosystem models, which simulate biogeochemical processes in the ocean, are a representative example. In this paper, we introduce a surrogate-based optimization (SBO) methodology where the expensive fine model is replaced by its fast and yet reasonably accurate surrogate. As a case study, we consider a representative of the class of one-dimensional marine ecosystem models. The surrogate is obtained from a temporarily coarser discretized physics-based low-fidelity (or coarse) model. and a multiplicative response correction technique. In our previous work, a basic formulation of this surrogate was sufficient to create a reliable approximation, yielding a remarkably accurate solution at low computational costs. This was verified by model generated, attainable data. The application on real data is covered in this paper. Enhancements of the basic formulation by utilizing additionally fine and coarse model sensitivity information as well as

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trust-region convergence safeguards allow us to further improve the robustness of the algorithm and the accuracy of the solution. The trade-offs between the solution accuracy and the extra computational overhead related to sensitivity calculation will be addressed. We demonstrate that SBO is able to yield a very accurate solution at still low computational costs. The optimization process – when compared to the direct fine model optimization – is significantly speed up to about 85%.

Keywords: Climate models, marine ecosystem models, surrogate-based optimization, parameter optimization, response correction, efficient optimization, surrogate

1. Introduction

Numerical simulations play a key role to simulate and predict processes in the earth's climate system, ranging from fluid mechanics, as in the atmosphere and ocean, to bio- and biochemical interactions, e.g., in marine or other type of ecosystems. The underlying models are typically given as time-dependent partial differential or differential algebraic equations (PDEs/DAEs) [10, 17, 19].

Since many important processes are non-linear, the numerical effort to simulate the whole or parts of the climate system with a satisfying accuracy and resolution is quite high. This motivates the development and use of reduced order models by e.g. coarser discretizations (in time and/or space) or by parametrizations to reduce the system size and thus the computational effort [19]. Through those parametrizations, several additional parameters enter the system. Many of them are not known beforehand and not directly measurable. Before a transient simulation of a model (e.g., used for predictions) is possible, the latter has to be calibrated and validated w.r.t. measurement data, i.e., relevant unknown parameters have to be identified using large-scale optimization methods. Growth and dying rates in marine ecosystem models [7, 26], one of which is taken as a test case for the proposed optimization methodology, are examples for such unknown parameters. Marine ecosystem models describe photosynthesis and other biogeochemical processes in the marine ecosystem that are important, e.g., to compute and predict the oceanic uptake of carbon dioxide (CO_2) as part of the global carbon cycle [26].

The mathematical task of parameter optimization can be classified as a least-squares type optimization or inverse problem [2, 3, 31]. This optimization (or calibration) process requires a substantial number of (typically expensive) function and optionally sensitivity or even Hessian matrix evaluations.

Straightforward attempts by employing the *high-fidelity* or *fine* model under consideration directly in an optimization loop using conventional optimization algorithms are therefore tedious or even infeasible, especially when using traditional, gradient-based techniques. The need for an accelerated optimization process, which especially becomes important while handling complex three-dimensional models, becomes critical.

Surrogate-based optimization (SBO) addresses this issue by shifting the computational burden from the accurate and expensive high-fidelity model to its fast but yet reasonably accurate surrogate. More specifically, the idea of SBO is to replace the fine model in the optimization process in the sense of providing predictions of the model optimum. The surrogate can be created by approximating sampled fine model data (so-called *function-approximation surrogates*, see [23, 28, 29]) or by employing a physics-based *low-fidelity* or *coarse* model, a computationally cheap representation of the fine model. The latter approach is used in this paper. Since the accuracy of the coarse model is usually not sufficient to directly use the latter in an optimization loop, it is often necessary to use suitable alignment/correction techniques to reduce the misalignment between the coarse and fine model responses. Popular correction/alignment techniques include response correction [30] and space mapping [1]. Surrogate-based optimization is widely and very successfully used in engineering sciences, compare for example [1, 9, 15, 23].

As a case study, in order to investigate the applicability of a SBO methodology to the optimization of marine ecosystem models, we consider a representative of the class of one-dimensional models. Clearly, the computational effort in a one-dimensional simulation is significantly smaller than in the three-dimensional case. However, since biochemistry mainly happens locally in space and since the complexity of the biogeochemical processes included in this specific model is high, this model serves as a good test example for the applicability of SBO approaches, before considering computationally more expensive three-dimensional models.

One straightforward way to introduce a physics-based coarse model is to reduce the spatial