

Entirely Exponential-Type Scheme (E2S) for Optimization Problems with Singularly Perturbed ODE Constraints: The Model Problem

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Abstract. We found that no convergence to the correct solution can happen when a popular method is applied to discretize the derivative appearing in the objective function for optimization problems with singularly perturbed ODE constraints. The non-convergence mentioned above can occur even if the error bound of the numerical solution of the state equation has nothing to do with the small parameter. We disclose that the underlying reason for non-convergence to the correct solution is an inaccurate derivative calculation in the objective function for a model problem, which is solvable mathematically. To ensure correct convergence regardless of the small parameter, we propose an entirely exponential-type scheme for solving the optimization problem, in which an exponential-type scheme is used for the derivative in the objective function, together with an exponential-type finite difference scheme for the state equation. Both theoretical analysis and numerical experiments can verify the correct convergence of E2S in solving the singularly perturbed equation-constrained optimization problem.

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1. Introduction

PDE-constrained optimization problems are of great significance in the fields of mathematical physics and engineering [1, 3, 5, 12, 16]. Their numerical studies involve many aspects, including optimality theory, discrete methods for optimization problems, and others. Such problems exhibit substantial challenges in both theoretical analysis

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and numerical computation. In theoretical analysis, it is essential to consider

- (i) the properties related to the regularity of state equations,
- (ii) the existence and uniqueness of optimization solutions,
- (iii) the first-order optimality conditions and second-order sufficient conditions.

In numerical computation, researchers mainly focus on the effects of numerical methods for partial differential equations (PDEs) on optimal solutions, while the effects of numerical methods for the objective function receive less attention. In this paper, we main focus on the effects of the combined schemes of the PDE and the objective function on the optimization solutions for a special constrained optimization problem.

Among the PDE-constrained optimization problems, there is a special kind where the state equation is singularly perturbed and the objective function is equipped with the product of a small parameter with a partial derivative. For example, the optimization problem of cooling and drag reduction near the wall under the constraints of the steady-high Reynolds number Navier-Stokes (N-S) equations can be clearly stated mathematically as the singularly perturbed equation-constrained optimization problem (SPE-COP). Such an optimization problem deviates from the general PDE-constrained optimization problem in two facets. On one hand, the state equation has boundary layer phenomena. On the other hand, the optimization objective takes the form of small perturbation parameter multiplied by the gradient of the physical quantity. The theoretical analysis and numerical simulation of SPE-COP are very challenging and meaningful. In terms of numerical study, we found that the discretization of the state equation and objective function hold significant importance in accurately calculating the optimal solution.

For the state equation of singular perturbation, it is known that the classical upwind difference (UD) scheme is not uniformly convergent in the discrete maximum norm if the given problem features a typical exponential boundary. Numerical errors inside the boundary layer have a significant impact on numerical solutions in that region. Many researchers have considered the numerical methods of singularly perturbed differential equations [7–9, 14, 15], such as various finite difference methods, finite volume methods, finite element methods based on special grids and discretization. Among them, the Il'in-Allen-Southwell (IAS) scheme [6, 10, 13, 14] is an exponentially fitted finite difference scheme based on uniform grids for second-order singularly perturbed differential equations, which was originally derived by Allen and Southwell [2] and later proved uniform convergence by Il'in [6].

For the objective function, the classical difference discretization (CDD) incurs a significant error when calculating the derivative value at the boundary layer, even with an analytical solution for the state equation. Moreover, it also leads to optimization failure, i.e., non-convergence to the correct solution, as one will see later in a simple 1D problem.

In this paper, we shall propose an exponential-type scheme (ETS) to efficiently compute the first-order derivative of the objective function, with the ETS derived from