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Variational approach and Euler's integrating factors for environmental studies

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ABSTRACT

We are promoting the use of variational principles as some generalizing idea that allows us to create consistent approximations of mathematical models. In this paper, we formulate a computing technology to solve direct and inverse problems of atmospheric dynamics and chemistry. For the implementation, we use functional decomposition methods, splitting techniques, and integrating factors designed as the solutions of some adjoint problems.

One of the main purposes of the paper is to relate the theory of approximation with the concept of Eulerian integrating factors that plays the fundamental role in the theory of differential equations. We demonstrate the utility and versatility of the concept applying it to solve the systems of differential equations of convection–diffusion (with dominant convection) and stiff systems of kinetic equations. To identify the prospects of our approach, we briefly introduce how to use integrating factors in the case of unstructured grids.

1. Introduction

In recent years, researchers have been actively developing integrated systems of mathematical models in which the mechanisms of transport and transformation of various substances in the gas and aerosol states are considered along with hydrodynamic processes in the atmosphere [1–6]. In these models, the system of nonstationary convection–diffusion–reaction equations describes the physical and chemical processes. To reproduce their behavior adequately, we need to have universal and computationally efficient methods of constructing numerical models and algorithms of their implementation.

There exist several approaches to constructing numerical algorithms to solve linear and nonlinear problems of mathematical physics including the problems of convection–diffusion type. Finite difference methods, variational finite element methods (FEM) and discontinuous Galerkin methods (DG) are most advanced and theoretically substantiated. Boundary element methods (BEM), which are also variational, are an alternative and, in fact, a very useful addition to the above methods. Detailed descriptions of major points of all these methods, with examples of solving practical problems, and an extensive literature, can be found in numerous textbooks on calculation methods (see, for instance, [7–13]).

For chemical problems, it is well-known that multistep implicit methods are most suitable for solving stiff systems of differential equations. These are Runge–Kutta methods with modifications of the iterative Newton's method for nonlinear systems, Gear and Rosenbrock methods, as well as combined Runge–Kutta and Rosenbrock methods, quasi-stationary concentration methods, etc. Some theoretical and computational aspects of these methods are described in detail in [14–17]. Various algorithms and program packages specially designed for problems of atmospheric chemistry (see, for instance, [1–4,18–20] and the references therein) have been developed. From the point of view of computational efficiency, the most

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time-consuming element of technologies with implicit numerical schemes is inverting, at each calculation step, the preconditioned matrices of large size containing the Jacobi matrices of linearized systems of equations. Another difficulty is the requirement that the sought-for functions be positive in the process of calculations.

The modern tendencies in the development of environmental prediction are toward solving inverse problems with assimilation of observation data. In comparison with direct problems, these problems need qualitatively new methods of direct and inverse simulation.

One of the main purposes of the paper is to relate the theory of approximation with the concept of Eulerian integrating factors that are fundamental to the theory of differential equations.

A variational method presented in this paper for constructing discrete–analytical numerical schemes to solve problems of mathematical physics employs the fundamental idea of Euler's integrating factors [21]. L. Euler proposed this idea to reduce the order of ordinary differential equations. The classical monograph [22] presents a detailed description of this approach using Lagrange's identity and Green's second formula for ordinary differential equations of arbitrary order (see [23]). Papers [24,25] give a description of Riemann's method, in which the solutions of the adjoint equations were used for 2D hyperbolic problems.

We use the idea of adjoint integrating factors within the framework of a variational principle for solving direct and inverse problems of the dynamics of atmosphere, ocean, and environmental protection [26–29]. The major elements in such models are similar in structure to operators of the convection–diffusion–reaction type.

In this paper, we present a variational method for constructing consistent numerical schemes and algorithms. First, we build a global variational principle for a generalized description of the original problem. Then we produce a decomposition of the functional of this principle. To this goal, we base on the additive properties of integration and differentiation operators included in the definition of the functional and obtain the complete approximation of the functional. Such an approach allows us to create the consistent description of convection–diffusion and transformation operators as the parts of general system. Here, for the convenience of algorithmic implementation, we represent multi-dimensional system in the frames of integral identity as the sum of the two groups of terms, in which there are locally one-dimensional objects. They are: (a) locally one-dimensional with respect to one of three spatial variables for convection–diffusion operators, and (b) locally one-dimensional in time in transformation operators. Since our problem is four-dimensional one, a parametric dependence from the other three coordinates remains in each of the terms. To approximate one-dimensional objects, we apply the idea of integrating factors. The solutions to some specific local adjoint problems play the roles of these factors. Finally, approximating all the terms of the integral identity for parametric variables, we obtain a complete discrete analog of the functional of our variational principle.

This approach is efficient in multi-dimensional cases where some variational principles are used in combination with decomposition and splitting methods to generate hybrid methods for mathematical simulation of processes of different scales and dimensions employing the best properties of the above-mentioned major branches of numerical analysis.

It should be emphasized, that the problems, which we solve for description of the dynamics and quality of the atmosphere, are the problems with dominant convection. With the help of integrating factors and associated problems, we build unconditionally monotone, stable, implicit discrete–analytical schemes, which are locally accurate even if diffusion degenerates.

Considerable difficulty in modern numerical models is solving problems in spatial domains of complex configuration. This topic is closely related to the construction of grids and the subsequent approximation of huge models for these grids. Currently, for global and regional problems of the dynamics and chemistry of the atmosphere, the grids with a quasi-uniform resolution are predominantly used. There are some kinds of such grids for sphere: latitude–longitude, triangular icosahedral, "cubic sphere", as well as combined latitude–longitude Yin-Yang grid, in which the polar regions are excluded [30]. Our approach with integrating factors and adjoint equations gives the possibility of constructing new hybrid approximations effectively implemented on such quasi-regular and unstructured grids.

Let us list some of new elements of our approach presented in the paper.

One of the main results is a new version of the variational principle for convection–diffusion–reaction problems using the concept of integrating factors combined with specific adjoint technique. A general scheme of functional decomposition of an integral identity of the variational principle for the description of the mathematical model taking into account an additive representation of the major model objects is formulated in Section 3. The universal scheme of the algorithms with integrating factors for the linear differential operators of the order $M \geq 1$ (M is the order of the highest derivative) is described in Section 5. The schemes for convection–diffusion equation with the use of the first and second-order backward difference formulas in time are constructed in Section 6. They have the properties of unconditional monotony and L-stability. Approximations of four types of boundary conditions such as Dirichlet, Neumann, mixed and periodic are presented in Section 6.2. In Section 7, the scheme for the problem of degenerate diffusion (convective transport equation) is given. The quality of the scheme is demonstrated by Godunov's test problem (Section 7.1). In Section 10, we have a new version of the finite element method for unstructured grids based on adjoint integrating factors.

One of the main theoretical results of our studies is development of the variational technique, in which the severity of constructing approximations for the operators defined on spaces of the state functions of original problem is moved on fundamental solutions of the corresponding homogeneous adjoint problems. For this purpose, the concept of adjoint integrating factors is essentially used.

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