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Application of variational principles and adjoint integrating factors for constructing numerical GFD models

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The proposed method is considered on an example of hydrothermodynamics and atmospheric chemistry models [1,2]. In the development of the existing methods for constructing numerical schemes possessing the properties of total approximation for operators of multiscale process models, we have developed a new variational technique, which uses the concept of adjoint integrating factors.

The technique is as follows. First, a basic functional of the variational principle (the integral identity that unites the model equations, initial and boundary conditions) is transformed using Lagrange's identity and the second Green's formula. As a result, the action of the operators of main problem in the space of state functions is transferred to the adjoint operators defined in the space of sufficiently smooth adjoint functions. By the choice of adjoint functions the order of the derivatives becomes lower by one than those in the original equations. We obtain a set of new balance relationships that take into account the sources and boundary conditions. Next, we introduce the decomposition of the model domain into a set of finite volumes. For multi-dimensional non-stationary problems, this technique is applied in the framework of the variational principle and schemes of decomposition and splitting on the set of physical processes for each coordinate directions successively at each time step. For each direction within the finite volume, the analytical solutions of one-dimensional homogeneous adjoint equations are constructed. In this case, the solutions of adjoint equations serve as integrating factors. The results are the hybrid discrete-analytical schemes. They have the properties of stability, approximation and unconditional monotony for convection-diffusion operators. These schemes are discrete in time and analytic in the spatial variables. They are exact in case of piecewise-constant coefficients within the finite volume and along the coordinate lines of the grid area in each direction on a time step. In each direction, they have tridiagonal structure. They are solved by the sweep method. An important advantage of the discrete-analytical schemes is that the values of derivatives at the boundaries of finite volume are calculated together with the values of the unknown functions. This technique is particularly attractive for problems with dominant convection, as it does not require artificial monotonization and limiters.

The same idea of integrating factors is applied in temporal dimension to the stiff systems of equations describing chemical transformation models [2].

The proposed method is applicable for the problems involving convection-diffusion-reaction operators.

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