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Variational methods for direct/inverse problems of atmospheric dynamics and chemistry

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We present a variational approach for solving direct and inverse problems of atmospheric hydrodynamics and chemistry. It is important that the accurate matching of numerical schemes has to be provided in the chain of objects: direct/adjoint problems – sensitivity relations – inverse problems, including assimilation of all available measurement data. To solve the problems we have developed a new enhanced set of cost-effective algorithms.

The matched description of the multi-scale processes is provided by a specific choice of the variational principle functionals for the whole set of integrated models. Then all functionals of variational principle are approximated in space and time by splitting and decomposition methods.

Such approach allows us to separately consider, for example, the space-time problems of atmospheric chemistry in the frames of decomposition schemes for the integral identity sum analogs of the variational principle at each time step and in each of 3D finite-volumes. To enhance the realization efficiency, the set of chemical reactions is divided on the subsets related to the operators of production and destruction. Then the idea of the Euler's integrating factors is applied in the frames of the local adjoint problem technique [1]-[3]. The analytical solutions of such adjoint problems play the role of integrating factors for differential equations describing atmospheric chemistry. With their help, the system of differential equations is transformed to the equivalent system of integral equations. As a result we avoid the construction and inversion of preconditioning operators containing the Jacobi matrixes which arise in traditional implicit schemes for ODE solution. This is the main advantage of our schemes.

At the same time step but on the different stages of the "global" splitting scheme, the system of atmospheric dynamic equations is solved. For convection – diffusion equations for all state functions in the integrated models we have developed the monotone and stable discrete-analytical numerical schemes [1]-[3] conserving the positivity of the chemical substance concentrations and possessing the properties of energy and mass balance that are postulated in the general variational principle for integrated models. All algorithms for solution of transport, diffusion and transformation problems are direct (without iterations).

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