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Variational inequality approach to enforcing the non-negative constraint for advection-diffusion equations

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Abstract. Predictive simulations are crucial for the success of many subsurface applications, and it is highly desirable to obtain accurate non-negative solutions for transport equations in these numerical simulations. To this end, optimization-based methodologies based on quadratic programming (QP) have been shown to be a viable approach to ensuring discrete maximum principles and the non-negative constraint for anisotropic *diffusion* equations. In this paper, we propose a computational framework based on the variational inequality (VI) which can also be used to enforce important mathematical properties (e.g., maximum principles) and physical constraints (e.g., the non-negative constraint). We demonstrate that this framework is not only applicable to diffusion equations but also to non-symmetric advection-diffusion equations. An attractive feature of the proposed framework is that it works with with any weak formulation for the advection-diffusion equations, including single-field formulations, which are computationally attractive. A particular emphasis is placed on the parallel and algorithmic performance of the VI approach across *large-scale* and *heterogeneous* problems. It is also shown that QP and VI are equivalent under certain conditions. State-of-the-art QP and VI solvers available from the PETSc library are used on a variety of steady-state 2D and 3D benchmarks, and a comparative study on the scalability between the QP and VI solvers is presented. We then extend the proposed framework to transient problems by simulating the miscible displacement of fluids in a heterogeneous porous medium and illustrate the importance of enforcing maximum principles for these types of coupled problems. Our numerical experiments indicate that VIs are indeed a viable approach for enforcing the maximum principles and the non-negative constraint in a large-scale computing environment. Also provided are Firedrake project files as well as a discussion on the computer implementation to help facilitate readers in understanding the proposed framework.

A list of abbreviations

ABC	Arnold-Beltrami-Childress
CG	Conjugate Gradient method
DG	Discontinuous Galerkin
GAL	(Continuous) Galerkin
GMRES	Generalized Minimal Residual method
KSP	Krylov subspace iterative solver

Key words and phrases. anisotropy; variational inequalities; quadratic programming; non-negative solutions; maximum principles; parallel computing; advection-diffusion equations; miscible displacement.