Monotonicity recovering postprocessing of FE solutions

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Simulation of transport phenomena based on advection-diffusion equation is very popular in many engineering applications. Non-monotonicity of the numerical solution is the typical drawback of the conventional methods of approximation, such as finite elements (FE), finite volumes, and mixed finite elements. The problem of monotonicity is particularly important in cases of highly anisotropic diffusion tensors or distorted unstructured meshes. For instance, in the nuclear waste transport simulation, the non-monotonicity results in the presence of negative concentrations which may lead to unacceptable concentration and chemistry calculations failure. Another drawback of the conventional methods is a possible violation of the discrete maximum principle, which establishes lower and upper bounds for solution.

We suggest here a least-change correction to the available FE solution $\bar{x} \in R^n$. This postprocessing procedure is aimed on recovering the monotonicity and some other important properties that may not be exhibited by $\bar{x}$. The mathematical formulation of the postprocessing problem is reduced to the following convex quadratic programming problem

$$\begin{array}{ll} \min & \|x - \bar{x}\|^2 \\ \text{s.t.} & Mx \geq 0, \\ & l \leq x \leq u, \\ & e^T x = m. \end{array} \tag{1}$$

The set of constraints $Mx \geq 0$ represents here the monotonicity requirements. It establishes relations between some of the adjacent mesh cells in the form $x_i \leq x_j$, which relates cells i and j. The corresponding row of the matrix M is composed mainly of zeros, but its ith and jth elements, which are equal to -1 and $+1$, respectively. The set of constraints $l \leq x \leq u$ originates from the discrete maximum principle. In the last constraint, $e = (1, 1, \ldots, 1)^T \in R^n$. It formulates the conservativity requirement.

The postprocessing based on (1) is typically a large scale problem. We introduce here algorithms for solving this problem. They are based on the observation that, in the presence of the monotonicity constraints only, problem (1) is the classical monotonic regression problem, which can be solved efficiently by some of the available monotonic regression algorithms. This solution is used then for producing the optimal solution to problem (1) in the presence of all the constraints. We present results of numerical experiments to illustrate the efficiency of our approach.