"New monotone scheme for diffusion type problems on unstructured meshes"

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Summary

The discretization methods used in existing simulations of a subsurface flow fail to preserve positivity of a continuum solution of the pressure equation when the porous media is heterogeneous and anisotropic. A negative discrete solution implies non-physical Darcy velocities and hence wrong prediction of a contaminant transport. In our research we study new monotone finite volume discretization methods that guarantee positivity of the discrete solution for unstructured meshes and strongly heterogeneous anisotropic diffusion tensors.

Predictive numerical simulations of subsurface processes require not only more sophisticated physical models but also more accurate and reliable discretization methods for these models. In [1] we study a new monotone finite volume scheme for diffusion problems with a heterogeneous anisotropic material tensor. Development of a new discretization scheme should be based on the requirements motivated by both practical implementation and physical background. This scheme must

- be locally conservative;
- be monotone, in particular preserve positivity of the differential solution;
- be applicable to unstructured, anisotropic, and severely distorted meshes;
- allow arbitrary diffusion tensors;
- result in sparse systems with a minimal number of non-zero entries;
- have higher than the first-order accuracy for smooth solutions.

The discretization methods used in existing simulations, such as Mixed Finite Element (MFE) method, Finite Volume (FV) method, Mimetic Finite Difference (MFD) method, Multi Point Flux Approximation (MPFA) method, satisfy most of these requirements except the **monotonicity**. They fail to preserve positivity of a continuum solution when the diffusion tensor is heterogeneous and anisotropic or the computational mesh is strongly perturbed, see Figure. In simulations of a subsurface transport, a negative discrete solution of the pressure equation implies non-physical Darcy velocities and hence wrong prediction of a contaminant transport.

Recently, the nonlinear monotone scheme has been suggested by C. Le Potier in [2]. We studied schemes based on the nonlinear flux formula proposed in [2]. The diffusion flux is approximated at the middle of each mesh edge using a weighted difference of
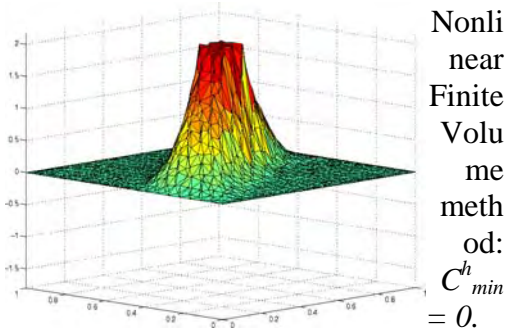
concentrations C at reference points in two neighboring cells. Nonlinearity of the method comes from the fact that these weights depend on a concentration at the edge
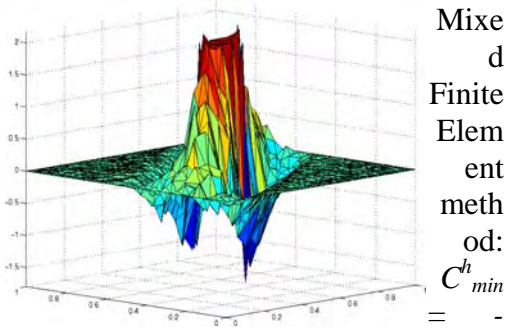
Mixed Finite Element method: $C^h_{min} = -1.7$

Nonlinear Finite Volume method: $C^h_{min} = 0$.

Profile of discrete solution $C^h(x,y)$ on the distorted triangular grid. Domain: unit square with the hole in the center. Problem: diffusion equation with highly anisotropic tensor. Ratio of tensor's eigenvalues is 10^3. Analytical solution satisfies maximum principle $0 \leq C\,x,y \leq 2$. The MFE method produces non-physical solution with strong negative values.

vertices. The position of the reference point depends on the geometry of a cell and a value of the diffusion tensor. For isotropic diffusion tensors and a triangular cell , the center of the inscribed circle is the acceptable position for the reference point. We rectified the Le Potier's scheme for the case of unstructured triangulations and full diffusion tensors by giving correct positions of reference points. To improve robustness of the scheme, we proposed an alternative interpolation technique [3]. We gave the first proof of scheme monotonicity for the steady diffusion equation. We studied numerically important features of the scheme such as violation of the discrete maximum principle and impact of the diffusion anisotropy on the scheme convergence. We extended the scheme to shape regular polygonal meshes and heterogeneous isotropic diffusion tensors.

The nonlinear finite volume method results in a sparse system whose dimension is equal to the number of mesh cells. For triangular meshes, the matrix of this system has at most four non-zero elements in each row. To solve the nonlinear algebraic problem we use the Picard iterative method which guarantees monotonicity of the discrete solution for all iterative steps.

The computational results demonstrate the flexibility and accuracy of the scheme. For sufficiently smooth solutions, we achieve the
second-order convergence for scalar unknowns and at least the first-order for the flux in a mesh-dependent L_2-norm. For non-smooth, highly anisotropic solutions we observe at least the first-order convergence for both unknowns.

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