Nonlinear Monotone FV Schemes for Radionuclide Geomigration and Multiphase Flow Models

Ivan Kapyrin, Kirill Nikitin, Kirill Terekhov and Yuri Vassilevski

Abstract We present applications of the nonlinear monotone finite volume method to radionuclide transport and multiphase flow in geological media models. The scheme is applicable for full anisotropic discontinuous permeability or diffusion tensors and arbitrary conformal polyhedral cells. We consider two versions of the nonlinear scheme: two-point flux approximation preserving positivity of the solution and compact multi-point flux approximation that provides discrete maximum principle. We compare the new nonlinear schemes with the conventional linear two-point and multi-point (O-scheme) flux approximations. Both new nonlinear schemes have compact stencils and a number of important advantages over the traditional linear discretizations. Two industrial applications are discussed briefly: radionuclides transport modeling within the radioactive waste safety assessment and multiphase flow modeling of oil recovery process.

Ivan Kapyrin
Institute of Numerical Mathematics, Gubkina 8, Moscow, Russia,
Institute of Nuclear Safety, B.Tulskaya 52, Moscow, Russia, e-mail: ivan.kapyrin@gmail.com

Kirill Nikitin
Institute of Numerical Mathematics, Gubkina 8, Moscow, Russia,
Institute of Nuclear Safety, B.Tulskaya 52, Moscow, Russia, e-mail: nikitin.kira@gmail.com

Kirill Terekhov
Institute of Numerical Mathematics, Gubkina 8, Moscow, Russia, e-mail: kirill.terehov@gmail.com

Yuri Vassilevski
Institute of Numerical Mathematics, Gubkina 8, Moscow, Russia,
Moscow Institute of Physics and Technology, Institutski 9, Dolgoprudny, M.R., Russia, e-mail: yuri.vassilevski@gmail.com

Introduction

A simple and accurate conservative method applicable to general conformal meshes and full anisotropic tensor permeability coefficients, is much-in-demand among engineers. The maximum principle is one of the important properties of solutions of partial differential equations (PDEs) such as the diffusion or heat equation. Its discrete counterpart is a very desirable property to have in a numerical scheme. Unfortunately, the schemes satisfying the discrete maximum principle (DMP) impose severe limitations on mesh regularity [6] and problem coefficients. Violation of the DMP leads to various numerical artifacts, such as heat flow from a cold material to a hot one, that can be amplified by physics non-linearity.

The classical two-point finite volume (FV) scheme for diffusion problems defines a two-point flux approximation (TPFA) across a mesh face as a difference of two concentrations at neighboring cells times a transmissibility coefficient. It results in a system of algebraic equation with an M-matrix with diagonal dominance in rows, which implies immediately the discrete maximum principle [15]. However, accuracy of this scheme depends on mesh geometry and mutual orientation of mesh faces and principle directions of the diffusion tensor. More precisely, the co-normal vector for a face must be collinear to the vector connecting neighboring collocation points, which is clearly the impossible requirement for arbitrary tensors and/or arbitrary polyhedral cells. The multi-point flux approximation (MPFA) scheme solves accuracy problem by using more than two points in the flux stencil [1] and a matrix of transmissibility coefficients. The MPFA scheme provides a second-order accurate approximation of concentrations but is often only conditionally stable and conditionally monotone [14].

A new research direction pioneered by Le Potier [7] uses a two-point flux stencil with two coefficients that depend on the concentrations in neighboring cells. Nonlinear FV schemes with TPFA proposed in [3, 5, 7, 9, 10, 13, 18] guarantee solution positivity on general meshes and for general tensor coefficients.

For general meshes and coefficients the DMP requires a nonlinear multi-point flux approximation. For diffusion problems, such schemes were proposed in [8, 19] using auxiliary unknowns at mesh vertices. Later an interpolation-free multi-point nonlinear approximation of diffusive fluxes was proposed for two-dimensional [11] and three-dimensional cases [2, 4]. The resulting scheme has the minimal stencil and reduces to the classical two-point FV scheme on Voronoi or rectangular meshes and for scalar (and, in a few cases, diagonal tensor) coefficients.

In this article, we present two our FV schemes for the steady-state diffusion equation with anisotropic coefficients: both schemes work on general polyhedral meshes and have a compact stencil, the first preserves non-negativity of the discrete solution and the second satisfies the DMP. We also briefly consider two applications of the nonlinear schemes to subsurface flows: simulation of radionuclides geomigration from a nuclear waste disposal and multiphase flow modeling of oil recovery process.

The paper outline is as follows. In Section 1 we introduce our nonlinear FV schemes for the steady-state diffusion equation. In Section 2 we present a new parallel toolkit and two industrial applications using the toolkit and the presented FV schemes.

1 Nonlinear finite volume methods

Let Ω be a three-dimensional polyhedral domain with boundary Γ. The mixed form of the diffusion equation for unknown concentration c with the Dirichlet boundary condition is as follows:

$$\begin{aligned} \mathbf{q} = -\mathbb{K}\nabla c, \quad \operatorname{div} \mathbf{q} &= f \qquad \text{in } \Omega, \\ c &= g \qquad \text{on } \Gamma. \end{aligned} \tag{1}$$

Here $\mathbb{K}(\mathbf{x})$ is a symmetric positive definite discontinuous (possibly anisotropic) diffusion tensor, $f(\mathbf{x})$ is a source term, and $g(\mathbf{x})$ is a boundary data.

A discretization scheme can have two additional properties: discrete maximum (or minimum) principle and non-negativity of the discrete solution. The minimum principle states that for $f \geq 0$ the concentration $c(\mathbf{x})$ satisfies:

$$\min_{\mathbf{x}\in\bar{\Omega}} c(\mathbf{x}) \geq \min\{0, \min_{\mathbf{x}\in\Gamma} g(\mathbf{x})\}.$$

The maximum principle is formulated similarly. In the following we shall refer to both principles as the maximum principle. Non-negativity is a weaker property which stems from the minimum principle: for non-negative f and g one has non-negative $c(\mathbf{x})$. A numerical scheme can provide non-negativity of c but violate the discrete maximum principle (DMP) and thus can produce oscillations.

The cell-centered FV scheme uses one degree of freedom, C_T, per cell T collocated at cell barycenter $\mathbf{x}_T$. Integrating the mass balance equation (1) over T and using the divergence theorem, we obtain:

$$\sum_{f\in\partial T} \sigma_{T,f}\, \mathbf{q}_f \cdot \mathbf{n}_f = \int_T f\,\mathrm{d}x, \qquad \mathbf{q}_f = \frac{1}{|f|}\int_f \mathbf{q}\,\mathrm{d}s, \tag{2}$$

where $\mathbf{q}_f \cdot \mathbf{n}_f$ is the total flux across face f, and $\sigma_{T,f}$ is either 1 or -1 depending on the mutual orientation of normal vector to face $\mathbf{n}_f$ and the outer normal to cell boundary $\mathbf{n}_T$.

Both nonlinear flux approximation schemes exploit the same idea of vector expansion. First we need to find a triplet of three vectors $\mathbf{t}_{1*}$ connecting $\mathbf{x}_{T_1}$ with other collocation points such that the co-normal vector $\ell_f = \mathbb{K}\cdot\mathbf{n}_f$ can be expanded

$$\ell_f = \alpha_{1a}\,\mathbf{t}_{1a} + \beta_{1b}\,\mathbf{t}_{1b} + \gamma_{1c}\,\mathbf{t}_{1c}, \qquad \alpha_{1a} \geq 0, \beta_{1b} \geq 0, \gamma_{1c} \geq 0, \tag{3}$$

where a, b, c are indexes of neighboring cells.

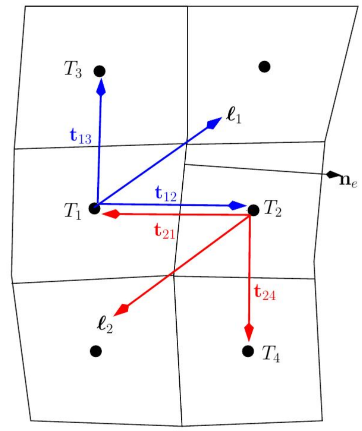

Fig. 1 Two representations of co-normal vector $\ell_1 = -\ell_2 = \mathbb{K} \cdot \mathbf{n}_e$ (2D example).

Since the flux normal component is the directional derivative along the co-normal vector ℓ_f, it can be represented as the sum of three directional derivatives along $\mathbf{t}_{1*}$ which are approximated by central differences:

$$(\mathbf{q}_f \cdot \mathbf{n}_f)_h^{(1)} = \alpha_{1a}\,(C_a - C_1) + \beta_{1b}\,(C_b - C_1) + \gamma_{1c}\,(C_c - C_1). \tag{4}$$

For the opposite co-normal vector $-\ell_e$ we have similar representation with another triplet and central differences, see Fig. 1 for the 2D example:

$$(-\mathbf{q}_f \cdot \mathbf{n}_f)_h^{(2)} = \alpha_{2k}\,(C_k - C_2) + \beta_{2l}\,(C_l - C_2) + \gamma_{2m}\,(C_m - C_2). \tag{5}$$

Our flux discretization is a linear combination of approximations (4) and (5) with coefficients μ_+ and μ_-. For the sake of approximation the linear combination should be convex:

$$\mu_+ + \mu_- = 1.$$

The second equation for $\mu_\pm$ is dictated by the goal of the method:

- To obtain the two-point discretization, we get rid of unwanted concentrations in the flux stencil:

$$\mu_+(\alpha_{1a}\,C_a + \beta_{1b}\,C_b + \gamma_{1c}\,C_c) - \mu_-(\alpha_{2k}\,C_k + \beta_{2l}\,C_l + \gamma_{2m}\,C_m) = 0.$$

- To provide the DMP, we balance the contributions of one-sided fluxes:

$$\mu_+(\mathbf{q}_f \cdot \mathbf{n}_f)_h^{(1)} = \mu_-(-\mathbf{q}_f \cdot \mathbf{n}_f)_h^{(2)},$$

  so that either (4) or (5) can be used in assembling the discrete fluxes in (2). This helps us to preserve compactness of the stencil for both cells T_1 and T_2 even with the multi-point fluxes (4), (5).

FV method with the nonlinear TPFA provides non-negativity of the discrete solution, whereas FV method with the nonlinear MPFA provides the DMP. In the case of $\mathbb{K}$-orthogonal mesh vectors $\mathbb{K}\mathbf{n}_f$ and $\mathbf{t}_{12}$ are collinear, both nonlinear flux approximations reduce to the conventional linear TPFA which provides at least first order accuracy. In general case, the linear TPFA may not provide approximation at all, whereas the linear MPFA may not provide the DMP or positivity.

2 Applications

Means for the development of parallel numerical models of complex phenomena on general polyhedral meshes are provided by data structures and algorithms from the open source package INMOST (Integrated Numerical Modelling Object-oriented Supercomputing Technologies) [17]. FV discretization assumes that the processor possessing a mesh cell has access to data in neighboring cells. If a cell adjoins to the boundary of the local submesh associated with a processor, some of its neighbors belong to other processors. For each local submesh we generate additional layers of ghost cells composed of these neighbors. The ghost cells contain exact copy of data of the associated normal cells. The main difference between the ghost cell and the normal cell is that the ghost cell data should be actualized after any update of the normal cell data. Actualization involves inter-processor communications that move the data from normal cells to their ghost copies. Mesh data structure implemented in INMOST allows simple design of a numerical scheme on each mesh cell and is very convenient even for single processor implementations. Both applications presented in this paper are built using INMOST toolkit.

First we consider application of the nonlinear FV schemes for the black-oil model [12, 16]. The black oil model describes the three-phase flow of water, oil and gas components in the underground reservoir. If the reservoir pressure drops below certain threshold, then oil is split into a liquid phase and gaseous phase at thermodynamic equilibrium. In this case the water phase does not exchange mass with the other phases, while the liquid and the gaseous phases exchange mass. The model consists of mass conservation equations for each of the components and Darcy's velocity equations for each phase:

$$\mathbf{u}_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha}\mathbb{K}\Big(\nabla p_\alpha - \rho_\alpha(p)\mathbf{g}\nabla z\Big), \quad \alpha = w,o,g, \tag{6}$$

where $\mathbb{K}$ is the absolute permeability tensor, z is the depth, $\mathbf{g}$ is the gravity term, p_α, S_α are *unknown* pressure and saturation, μ_α and $k_{r\alpha}$ are the formation viscosity and relative phase permeability, ρ_α are the densities at current conditions for the phase $\alpha = w,o,g$.

We use the fully implicit scheme in time and Newton method to solve the nonlinear system at each time step. Construction of the Jacobian matrix is based on partial derivatives with respect to primary variables (oil pressure p, water and gas

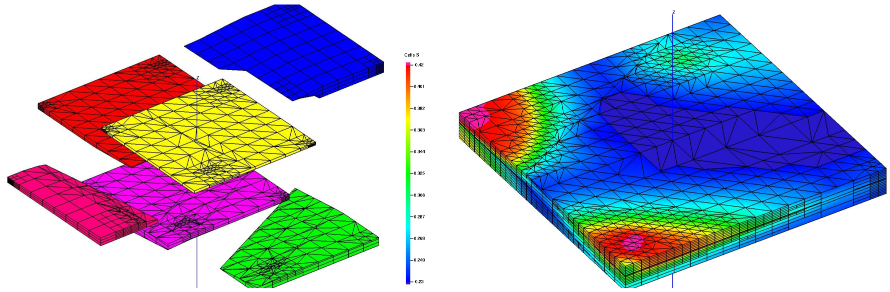

Fig. 2 Example of three-phase flow in heterogeneous media. Left: computational grid and geological layers. Right: water saturation field.

saturations S_w, S_g) of discrete Darcy fluxes. The latter are obtained either by the conventional linear TPFA or MPFA or by the nonlinear TPFA or MPFA presented above (the diffusion tensor should be replaced with absolute permeability tensor).

Dependence of the method coefficients on primary variables leads to the extension of the Jacobian stencil [12, 16]. For instance, in case of the nonlinear TPFA one has

$$-(\mathbb{K}\nabla p)_f^h \cdot \mathbf{n}_f = D_f^+(p)p_+ - D_f^-(p)p_-. \quad (7)$$

Coefficients $D_f^\pm$ must be differentiated as dependent on primary variables in neighboring cells: $\Delta D_p^\pm = \sum\limits_{T_i \in \Sigma_{T_*}} L_{p,i}^\pm \Delta p_{T_i}$, where $\Sigma_{T^*} = \Sigma_{T_+} \cup \Sigma_{T_-}$, $\Sigma_{T_\pm}$ is the set of cells forming the stencil for cell $T_\pm$, $L_{p,i}^\pm$ are the coefficients of differentiation. Wider stencil Σ_{T^*} for Jacobian results in more dense Jacobian matrix and more expensive Jacobian-vector multiplication and Jacobian preconditioning compared to the conventional linear TPFA. On the other hand, the linear TPFA is often inconsistent.

An example for three-phase water-flooding with several wells in heterogeneous media is shown in Fig. 2.

The second application of the nonlinear FV schemes is related to validation of safe subsurface disposal of radioactive wastes (RW). In this application two main tasks must be solved, the groundwater (GW) flow problem and the transport in porous media problem, which may be strongly coupled in some cases. The novel FV schemes are implemented within the code GeRa (Geomigration of Radionuclides). This code is developed to model the major significant processes for radwaste disposal safety: saturated and unsaturated flow, density-driven flow, reactive transport with decay, heat transport. The basis for all these numerical models are the discretizations of the diffusion and advection operators. The computational meshes are assumed arbitrary polyhedral. The code involves the triangular prismatic and the octree-hexahedral mesh generators. In the first generator the resulting meshes may contain triangular prisms, tetrahedra and pyramids. The octree hexahedral generator cuts and adapts the cells to the domain boundary and interfaces between geological layers leading to complicated polyhedral cells.

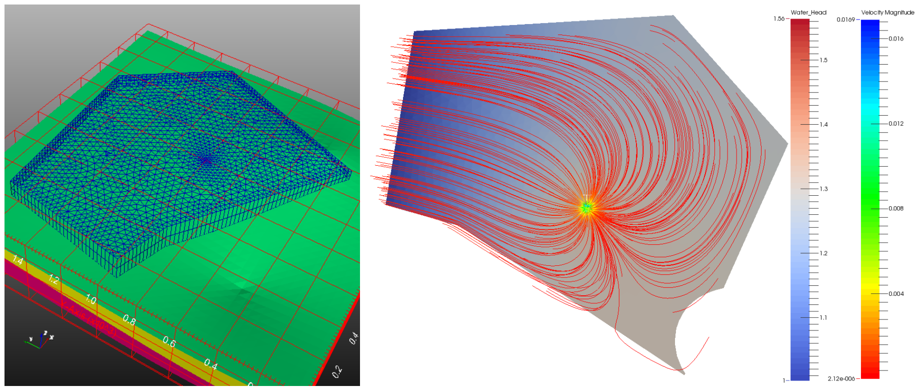

Fig. 3 Example problem: groundwater flow in a realistic heterogeneous media. Left: computational grid and geological layers. Right: pressure head and flow streamlines.

The GW flow problem may be solved by FV scheme with either the linear TPFA (may be inconsistent) and MPFA (may be non-monotone) or the nonlinear TPFA and MPFA (both consistent and monotone). For the temporal discretization the operator-splitting scheme or the implicit scheme may be used. The first one treats the advection operator explicitly and the diffusion operator implicitly. Advection may be modeled using the conventional first-order accurate FV scheme with piecewise-constant solution or the second-order accurate TVD-scheme with linear reconstruction of discrete solution on the cells. For the diffusion operator any of the four flux approximation schemes (linear/nonlinear TPFA/MPFA) may be applied. The implicit scheme solves the coupled advection-diffusion problem using the nonlinear FV method for diffusion and local linear solution reconstruction for advection.

Numerical experiments with GeRa show robustness of the nonlinear schemes: the resulting matrices are reasonably well conditioned and the solutions remain non-negative or satisfy the DMP. In case of large complicated grids and heterogeneous tensor coefficients the schemes provide the best solution, as they allow to solve efficiently the generated grid equations and they are consistent.

Fig.3 (left) presents a filtration model with three geological layers, single well and outflow boundary with a prescribed water head. Water head solution and flow streamlines obtained using the FV scheme with the nonlinear TPFA is shown on Fig.3 (right).

Acknowledgements This work has been supported in part by RFBR grants 12-01-33084, 14-01-00830, Russian Presidential grant MK-7159.2013.1, Federal target programs of Russian Ministry of Education and Science, ExxonMobil Upstream Research Company, and project “Breakthrough” of Rosatom.

References

1. Aavatsmark, I., Eigestad, G., Mallison, B., Nordbotten, J.: A compact multipoint flux approximation method with improved robustness. Num. Meth. for Part. Diff. Eqs. **24**(5), 1329–1360 (2008)
2. Chernyshenko, A.: Generation of adaptive polyhedral meshes and numerical solution of 2nd order elliptic equations in 3D domains and on surfaces. Ph.D. thesis, INM RAS, Moscow (2013)
3. Danilov, A., Vassilevski, Y.: A monotone nonlinear finite volume method for diffusion equations on conformal polyhedral meshes. Russ. J. Numer. Anal. Math. Modelling **24**(3), 207–227 (2009)
4. Gao, Z.M., Wu, J.M.: A small stencil and extremum-preserving scheme for anisotropic diffusion problems on arbitrary 2D and 3D meshes. J. Comp. Phys. **250**, 308–331 (2013)
5. Kapyrin, I.V.: A family of monotone methods for the numerical solution of three-dimensional diffusion problems on unstructured tetrahedral meshes. Doklady Mathematics **76**(2), 734–738 (2007)
6. Korotov, S., Křížek, M., Neittaanmäki, P.: Weakened acute type condition for tetrahedral triangulations and the discrete maximum principle. Math. Comp. **70**(233), 107–119 (2001)
7. LePotier, C.: Schema volumes finis monotone pour des operateurs de diffusion fortement anisotropes sur des maillages de triangle non structures. C. R. Acad. Sci. Paris, Ser. I **341**, 787–792 (2005)
8. LePotier, C.: Finite volume scheme satisfying maximum and minimum principles for anisotropic diffusion operators. In: R. Eymard, J.M. Hérard (eds.) Finite Volumes for Complex Applications, pp. 103–118 (2008)
9. Lipnikov, K., Svyatskiy, D., Vassilevski, Y.: Interpolation-free monotone finite volume method for diffusion equations on polygonal meshes. J. Comp. Phys. **228**(3), 703–716 (2009)
10. Lipnikov, K., Svyatskiy, D., Vassilevski, Y.: A monotone finite volume method for advection-diffusion equations on unstructured polygonal meshes. J. Comp. Phys. **229**, 4017–4032 (2010)
11. Lipnikov, K., Svyatskiy, D., Vassilevski, Y.: Minimal stencil finite volume scheme with the discrete maximum principle. Russ. J. Numer. Anal. Math. Modelling **27**(4), 369–385 (2012)
12. Nikitin, K., Terekhov, K., Vassilevski, Y.: A monotone nonlinear finite volume method for diffusion equations and multiphase flows. Comp. Geosci. (2013). DOI 10.1007/s10596-013-9387-6
13. Nikitin, K., Vassilevski, Y.: A monotone nonlinear finite volume method for advectiondiffusion equations on unstructured polyhedral meshes in 3d. Russ. J. Numer. Anal. Math. Modelling **25**(4), 335–358 (2010)
14. Nordbotten, J.M., Aavatsmark, I., Eigestad, G.T.: Monotonicity of control volume methods. Numer. Math. **106**(2), 255–288 (2007)
15. Stoyan, G.: On maximum principles for monotone matrices. Linear Algebra and Its Applications **78**, 147–161 (1986)
16. Terekhov, K., Vassilevski, Y.: Two-phase water flooding simulations on dynamic adaptive octree grids with two-point nonlinear fluxes. Russ. J. Numer. Anal. Math. Modelling **28**(3), 267–288 (2013)
17. Vassilevski, Y., Konshin, I., Kopytov, G., Terekhov, K.: INMOST - Program platform and graphic environment for development of parallel numerical models on general meshes (in Russian). Moscow university publishing, Moscow (2013)
18. Yuan, A., Sheng, Z.: Monotone finite volume schemes for diffusion equations on polygonal meshes. J. Comp. Phys. **227**(12), 6288–6312 (2008)
19. Yuan, G., Sheng, Z.: The finite volume scheme preserving extremum principle for diffusion equations on polygonal meshes. J. Comp. Phys. **230**(7), 2588–2604 (2011)