Journal of Computational Physics 252 (2013) 219–249

Contents lists available at SciVerse ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Monotonic solution of heterogeneous anisotropic diffusion problems

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ARTICLE INFO

Article history:
Received 14 February 2012
Received in revised form 1 March 2013
Accepted 6 June 2013
Available online 27 June 2013

Keywords:
Anisotropic diffusion
Heterogeneous medium
M-matrix
Delaunay mesh
Affine transformation
Edge swap

ABSTRACT

Anisotropic problems arise in various areas of science and engineering, for example groundwater transport and petroleum reservoir simulations. The pure diffusive anisotropic time-dependent transport problem is solved on a finite number of nodes, that are selected inside and on the boundary of the given domain, along with possible internal boundaries connecting some of the nodes. An unstructured triangular mesh, that attains the Generalized Anisotropic Delaunay condition for all the triangle sides, is automatically generated by properly connecting all the nodes, starting from an arbitrary initial one. The control volume of each node is the closed polygon given by the union of the midpoint of each side with the "anisotropic" circumcentre of each final triangle. A structure of the flux across the control volume sides similar to the standard Galerkin Finite Element scheme is derived. A special treatment of the flux computation, mainly based on edge swaps of the initial mesh triangles, is proposed in order to obtain a stiffness M-matrix system that guarantees the monotonicity of the solution. The proposed scheme is tested using several literature tests and the results are compared with analytical solutions, as well as with the results of other algorithms, in terms of convergence order. Computational costs are also investigated.

1. Introduction

Diffusion equation with anisotropic coefficients arises in many environmental topics, for example heat transfer, groundwater flow and transport problems, petroleum reservoir simulations, hydrodynamic simulations, semiconductor modelling, biology problems, ... These problems are characterized by a full rank diffusive tensor, that is diagonal only if the reference system is aligned with the principal direction of anisotropy [7].

Steady-state diffusion problems satisfy the Maximum Principle (MP), which states that the solution cannot have a maximum or a minimum within the interior of the domain. The numerical solvers are aimed at satisfying the discrete counterpart of the MP, the so-called Discrete Maximum Principle (DMP), computing numerical solution free of spurious oscillations. A number of sufficient conditions are given for a class of linear elliptic Partial Differential Equations (PDEs) problems [40,10,11,37,38]. The most common one is that the problem stiffness matrix is an M-matrix. An M-matrix is an irreducible matrix with diagonal positive coefficients, strictly diagonally dominant, or weakly diagonally dominant with strict inequality for at least one row and non-positive off-diagonal coefficients (see for example [27,33]).

Numerical schemes satisfying the DMP have been developed according to the sufficient conditions, by either properly discretizing the governing PDE or by employing a suitable mesh. Most success has been obtained in the isotropic case, where the diffusive tensor reduces to a scalar value. It has been shown [9,11] that the linear Finite Element (FE) method

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0021-9991/$ – see front matter
http://dx.doi.org/10.1016/j.jcp.2013.06.017

satisfies the DMP when the mesh is a simplicial and satisfies the so-called non-obtuse angle condition, that is the dihedral angles of all mesh elements are non-obtuse [27]. In the 2D and homogeneous case this condition can be replaced by the weaker Delaunay condition, that the sum of any pair of angles opposite to a common edge is less than or equal to π [26,39].

The anisotropic case is more difficult. Draganescu et al. [12] proved that the non-obtuse angle condition fails to guarantee DMP satisfaction in the anisotropic diffusion problem. Several techniques have been proposed: local adjustments have been apported to the underlying numerical scheme by Liska and Shashkov [30] and Kuzmin et al. [23], Sharma and Hammett [36] used a slop limiter function in the discretization of the governing PDEs, Li et al. [28] optimized a triangular mesh for an FE scheme in order to reduce unphysical oscillations. Le Potier [24,25] and Lipnikov et al. [29] proposed a non-linear first-order Finite Volume (FV) method that obtains an M-matrix on arbitrary meshes in cases of parabolic PDEs but does not satisfy DMP for steady-state problems. Mlacnik and Durlofsky [33] optimized the mesh for a Multi-Point Flux Approximation (MPFA) FV scheme. The authors in [33] map the anisotropic physical problem into an isotropic computational one and optimize in this space the original grid of the physical problem. They solve the isotropic problem in the computational space. The authors in [33] predict some limitations of the proposed optimization technique for heterogeneous media. Li and Huang [27] studied a linear FE method for steady-state diffusion problems and developed a generalization of the non-obtuse angle condition for anisotropic cases. The condition requires that the dihedral angles of all mesh elements, measured in a metric depending on the diffusive tensor, be non-obtuse. This requirement reduces to the non-obtuse angle condition for isotropic problems. The authors in [27] derived also a metric tensor to use for mesh generation based on the anisotropic non-obtuse angle condition. They adopted the so-called M-uniform mesh approach [20], where an anisotropic mesh is generated as an M-uniform mesh or a uniform mesh in the metric specified by a tensor. The metric tensor is symmetric and positive definite and provides information on the size, shape and orientation of mesh elements. M-uniform meshes generated with the metric tensor satisfy the anisotropic non-obtuse angle condition and are aligned with the diffusive tensor. Edwards and Zheng [13,14] developed a family of flux-continuous FV schemes for the solution of the general tensor pressure equation for subsurface flows. These schemes have full pressure continuity imposed across control volume faces, while the early family of flux-continuous schemes present a point-wise pressure and flux continuity. One of the main advantages of these schemes is that, due to continuity conditions, they retain a single degree of freedom per control volume. The authors in [14] assert that optimal support can be achieved by anisotropy favoring triangulation (where the sign of triangulation angle equals the sign of dominant principal direction angle). The authors in [14] triangulate each primal quadrilateral element of a structured grid, according to the local sign variation of the off-diagonal coefficient of the diffusive tensor. The scheme in [14] minimizes spurious oscillations in the computed solutions and leads to more robust quasi-positive families of flux-continuous schemes applicable to generally discontinuous full tensor problems.

Mesh locking effects may arise for strong anisotropy problems and can be experimentally observed when the discretization error does not decrease at the expected rate for the limiting anisotropy ratio [18,19]. Havu [18] and Havu and Pitkäranta [19] introduced a modification to the bilinear Galerkin scheme to solve locking problems for high anisotropy ratios. These modifications could alter the consistency of the original scheme for the isotropic case and factors tending to zero, proportionally to the expected convergence rate of the scheme, have to be introduced to recover the consistency. A completely different approach is to try to adapt the domain, or the mesh, or both, to anisotropy of the problem [2,3]. This approach can be used if the anisotropy ratio is constant. Manzini and Putti [31] presented a FV diamond scheme with second-order accurate spatial reconstruction for both tangential and normal cell interface gradients. This scheme maintains second-order convergence rate on unstructured triangular grids and the only locking effects appear for very high anisotropy ratios and for quasi-purely Neumann boundary conditions problems.

A novel methodology for the solution of the anisotropic heterogeneous diffusion problem is presented in this paper. The algorithm is aimed at solving the problem on a finite number of irregular points arbitrary selected within the computational domain, as done by the MPFA computational scheme. On the opposite, the resulting spatial discretization of the fluxes across the control volume is similar to the one occurring in the standard linear ($P1$) Galerkin FE scheme, the number of unknowns is restricted to the number of nodes and a procedure for flux coefficients formulation is suggested in order to prevent from spurious oscillations in the solution, that avoid mesh locking effects. This algorithm acts directly on the physical mesh and does not deal with computational space, nor with metrics depending on the anisotropy tensor and the number and the location of the given input nodes remain unchanged. The proposed approach represents a grid adjustment algorithm leading to anisotropy favoring grids, eventhough, unlike the optimal anisotropy favoring triangulation schemes proposed in [14], grid adjustment is obtained by checking the sign of the global stiffness coefficients.

The proposed algorithm is mainly finalized to the solution of the diffusive problem where tensor coefficients are constant in time, though it has been easily extended to problems, like groundwater simulations, with time-dependent coefficients, function of the velocity field [5]. In such problems (where diffusive coefficients depend on the velocity field), the proposed procedure has to be combined with methods achieving inter-element flux continuity, like Mixed Finite Elements and their hybridized formulation (see [32] and cited references), or MPFA schemes (see [33] and cited references). In [5] flux continuity has been obtained by a modified formulation of an element-lumping Mixed Hybrid FE scheme with unknowns number equal to the number of elements.

The work is organized as follows. In Section 2, the governing PDEs along with the initial and boundary conditions and the space/time integration leading to the solving system are presented. In Section 3, the computation of the so-called "anisotropic" circumcentre of each triangle and the general formulation of the flux coefficients are given. The flux coefficients are computed: in Section 4 for the case of isotropic medium and Generalized Delaunay (GD) mesh; in Section 5 for the case