Benchmark 3D: a linear finite element solver

Hanen Amor, Marc Bourgeois, and Gregory Mathieu

1 Introduction

In the present paper[1], we address some of the benchmark problems defined for the Finite Volume for Complex Applications conference (FVCA6 [1]). The tests, which are described in [2], consist in solving the following anisotropic diffusion problem :

$$\begin{cases} -\nabla.(K\nabla u) = \mathrm{f} & \text{on} \quad \Omega \\ \mathrm{u} = \overline{u} & \text{on} \quad \Gamma_d \end{cases} \tag{1}$$

where u is the unknown, Ω is in most cases a unit cube, $K : \Omega \rightarrow \mathbb{R}^{3\times3}$ is the diffusion tensor, f the source term and $\overline{u}$ the Dirichlet boundary conditions.
For this benchmark, the computations were performed with MELODIE (Modèle d'Evaluation à LOng terme des Déchets Irradiants Enterrés) software, which is devoted to simulate the migration of a plume of radionuclides in a 3-dimensional geological media.

2 Presentation of MELODIE

The MELODIE [3] software, is developped by IRSN, and constantly upgraded, to assess the long-term containment capabilities of radioactive waste repositories. This software is designed to model a disposal site taking into account all the main

[1]The model of this paper is provided by the benchmark organization. The results of this benchmark will be detailed and discussed by Florence HUBERT and Raphaële HERBIN in a paper gathering all the contributions.

Hanen Amor, Marc Bourgeois, and Gregory Mathieu
Institut de Radioprotection et de Sûreté Nucléaire - DSU/SSIAD/BERIS - BP 17 - 92262 Fontenay-aux-Roses Cedex,
email: {hanen.amor,marc.bourgeois,gregory.mathieu}@irsn.fr

J. Fořt et al. (eds.), *Finite Volumes for Complex Applications VI – Problems & Perspectives*, Springer Proceedings in Mathematics 4,
DOI 10.1007/978-3-642-20671-9_90,

physical and chemical characteristics of the disposal components. The model is adapted to large scales of time and space required for simulation.
The MELODIE software models water flow and the phenomena involved in the transport of radionuclides in saturated porous media in 2 dimensions and in 3 dimensions; physical and chemical interactions are represented by a retardation factor integrated in the computational equations. These equations are discretised using a so-called FVFE method -Finite Volume Finite Element-, which is based on a Galerkin method to discretise time and variables, together with a finite volume method using the Godunov scheme for the convection term. The FVFE method is used to convert partial differential equations into a finite number of algebraic equations that match the number of nodes in the mesh used to model the considered site. It also serves to stabilise the numerical scheme. The present benchmark adresses only diffusive problems, which are therefore solved by using a standard P1 finite element method.

3 Numerical results

Numerical results presented in that contribution concern the tests 1, 3 and 4. The error generated by the P1 method has been evaluated by defining the quantity: $e = u - u_h$, where u is the analytical solution and u_h is the numerical solution. Then the error can be computed as follows.

3.1 Discrete L^2 and H^1 norms

The continuous L^2 and H^1 norms of a function u are given by

$$\|u\|_{L^2(\Omega)} = \left(\int_\Omega u^2\right)^{1/2} \quad , \quad \|u\|_{H^1(\Omega)} = \|u\|_{L^2(\Omega)} + \|\nabla u\|_{L^2(\Omega)}$$

where Ω is an open bounded in $\mathbf{R}^3$. In most of the test cases, the domain Ω is a unit cube. To compute those norms, we perform the L^2 and H^1 semi-norm of the function u on a tetrahedron T:

$$\|u\|_{L^2(T)} = \left(\int_T u^2\right)^{1/2} \quad \text{and} \quad \|\nabla u\|_{H^1(T)} = \left(\int_T \nabla u^2\right)^{1/2}$$

The numerical quadrature used to approximate this integral, are given by the following formula:

- in the case where the values of the function u are known on the vertices

$$\int_T u^2 dx \backsimeq \frac{1}{4} V_T \sum_{i=1}^{4} u(\overline{s_i})^2$$

- in the case where values of the gradient of the function u are known on the centre of gravity

$$\int_T \nabla u.\nabla u dx \backsimeq V_T \nabla u(G_T).\nabla u(G_T)$$

The previous formula are adapted to calculate the relative L^2 norm of the error : erl2, the relative L^2 norm of a gradient of the error : ergrad and the relative L^2 norm of the energy norm : ener.

3.2 Expected results

• **Test 1 Mild anisotropy,** $u(x, y, z) = 1 + \sin(\pi x) \sin\left(\pi\left(y + \frac{1}{2}\right)\right) \sin\left(\pi\left(z + \frac{1}{3}\right)\right)$ min $= 0$, max $= 2$**, Tetrahedral meshes**

i	nu	nmat	umin	uemin	umax	uemax	normg
1	488	6072	7.69E-02	8.29E-02	1.935	1.935	1.791
2	857	11269	2.76E-02	2.83E-02	1.955	1.955	1.796
3	1601	21675	3.07E-02	3.07E-02	1.970	1.969	1.798
4	2997	41839	1.81E-02	1.77E-02	1.984	1.983	1.797
5	5692	81688	1.32E-02	1.37E-02	1.990	1.990	1.798
6	10994	160852	6.19E-03	6.49e-03	1.991	1.991	1.798

i	nu	erl2	ratiol2	ergrad	ratiograd	ener	ratioener
1	488	1.35E-02	-	2.32E-01	-	2.29E-01	
2	857	7.01E-03	3.531	1.17E-01	1.370	1.17E-01	1.362
3	1601	4.56E-03	2.052	1.14E-01	1.052	1.14E-01	1.082
4	2997	3.01E-03	1.998	1.13E-01	1.155	1.11E-01	1.170
5	5692	1.87E-03	2.219	9.03E-02	1.067	8.90E-02	1.035
6	10994	1.22E-03	1.941	7.05E-02	1.128	6.92E-02	1.148

• **Test 1 Mild anisotropy,** $u(x, y, z) = 1 + \sin(\pi x) \sin\left(\pi\left(y + \frac{1}{2}\right)\right) \sin\left(\pi\left(z + \frac{1}{3}\right)\right)$ min $= 0$, max $= 2$**, Kershaw meshes**

i	nu	nmat	umin	uemin	umax	uemax	normg
1	729	9097	1.34E-01	8.76E-02	1.833	1.883	1.834
2	4913	66961	3.12E-02	1.92E-02	1.955	1.970	1.797
3	35937	513313	8.55E-03	6.64E-03	1.988	1.992	1.783
4	274625	4018753	2.04E-03	1.92E-03	1.997	1.998	1.787

i	nu	erl2	ratiol2	ergrad	ratiograd	ener	ratioener
1	729	9.41E-02	-	8.88E-01	-	9.05E-01	-
2	4913	5.88E-02	0.737	5.70E-01	0.696	5.710E-01	0.723
3	35937	3.35E-02	0.849	3.49E-01	0.741	3.47E-01	0.750
4	274625	1.52E-02	1.158	1.99E-01	0.823	2.02E-01	0.793

• **Test 3 Flow on random meshes,** $u(x, y, z) = \sin(2\pi x) \sin(2\pi y) \sin(2\pi z)$**,** $\min = -1$, $\max = 1$**, Random meshes**

i	nu	nmat	umin	uemin	umax	uemax	normg
1	125	1333	-0.665	-0.338	0.685	0.363	6.004
2	729	9097	-0.885	-0.784	0.812	0.751	3.867
3	4913	66961	-0.970	-0.943	0.949	0.925	3.666
4	35937	513313	-0.988	-0.982	0.991	0.984	3.613

i	nu	erl2	ratiol2	ergrad	ratiograd	ener	ratioener
1	125	8.34E-01	-	9.77E-01	-	9.44E-01	-
2	729	1.97E-01	2.456	4.84E-01	1.193	4.17E-01	1.390
3	4913	5.16E-02	2.107	2.48E-01	1.051	2.10E-01	1.078
4	35937	1.33E-02	2.040	1.22E-01	1.067	1.03E-01	1.066

• **Test 4 Flow around a well, Well meshes,** $\min = 0$, $\max = 5.415$

i	nu	nmat	umin	uemin	umax	uemax	normg
1	1248	15886	0.189	0.189	5.360	5.360	1653.52
2	2800	37836	0.120	0.119	5.368	5.368	1634.57
3	5889	81531	0.078	0.076	5.345	5.345	1631.27
4	12582	178018	0.060	0.058	5.349	5.349	1628.68
5	25300	363768	0.046	0.045	5.377	5.377	1626.49
6	45668	662730	0.037	0.036	5.380	5.380	1625.64
7	79084	1154172	0.029	0.028	5.39	5.39	1624.98

i	nu	erl2	ratiol2	ergrad	ratiograd	ener	ratioener
1	1248	3.30E-03	-	1.52E-01	-	1.48E-01	-
2	2800	1.49E-03	2.941	9.83E-02	1.621	9.40E-02	1.703
3	5889	8.99E-04	2.058	6.93E-02	1.409	6.52E-02	1.472
4	12582	6.11E-04	1.522	5.36E-02	1.014	4.93E-02	1.104
5	25300	4.09E-04	1.722	4.26E-02	0.983	3.94E-02	0.960
6	45668	2.69E-04	2.130	3.50E-02	0.997	3.26E-02	0.954
7	79084	2.58E-04	0.224	3.05E-02	0.753	2.84E-02	0.751

4 Comments

The computations for the post-processing purpose of the relative L^2 error norm and the relative H^1 error semi-norm have been done using the continuous solution and a numerical quadrature rule presented in the section 3.1. As can be seen, for the test 1 using the Tetrahedral meshes, for the test 3 using the Random meshes and for the test 4 using the Well meshes, the theoretical results are recovered, since a convergence of order 2 for the L^2-norm and a convergence of order 1 for the H^1-norm are obtained. For the test 1 using the Kershaw meshes, the theoretical results are not recovered. In fact, a convergence of order 1 for the L^2-norm and a convergence of order 1/2 for the H^1-norm are obtained. Those decreases in the rates of convergence orders are due to the characteristics of the Kershaw meshes that present strong anisotropy.
In addition, FVFE method implemented in MELODIE is only available for tetrahedrons and conform meshes. In the benchmark, hexahedral meshes are divided in tetrahedrons without changing the number of vertices. For the tests 2 and 5, that kind of adaptation is not possible due to the specific shape of the meshes. It is the reason why those cases were not considered.
In this benchmark, the system obtained after assembling of the discretized equations on each element is linear. Within MELODIE, this linear system is solved by using a bi-conjugate gradient method with an incomplete Gauss-type preconditioning. That method is specifically suitable for resolution of non-symmetrical system. Thereby, among the solvers proposed in the benchmark, our choice was the Petsc bi-conjugate gradient (using various preconditioning) complying with the implemented method in MELODIE.

References

1. website : http://fvca6.fs.cvut.cz/
2. website : http://www.latp.univ-mrs.fr/latp_numerique/
3. website : http://www.irsn.fr/FR/Larecherche/outils-scientifiques/Codes-de-calcul/Pages/Le-logiciel-MELODIE-3133.aspxl

The paper is in final form and no similar paper has been or is being submitted elsewhere.