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Benchmark 3D: CeVeFE-DDFV, a discrete duality scheme with cell/vertex/face+edge unknowns

Yves Coudière, Florence Hubert and Gianmarco Manzini

1 Presentation of the scheme

The method that we investigate in this contribution was proposed by Y. Coudière and F. Hubert in [1] as a three-dimensional (3D) extension of the finite volume scheme previously studied by F. Hermeline in [4] and K. Domelevo and P. Omnès in [3]. This method belongs to the family of Discrete Duality Finite Volume (DDFV) methods, which can naturally handle anisotropic or non-linear problems on general distorted meshes.

In this benchmark paper, we present the results obtained by using the formulation in [1] and the variant for discontinuous permeabilities that is presented in the proceeding paper [2].

The DDFV method that we consider herein makes use of three polyhedral meshes for the solution approximation, denoted by $\mathcal{M}$, $\mathcal{N}$, $\mathcal{FE}$, and the mesh of diamonds for the solution gradient approximation, denoted by $\mathcal{D}$.

We denote the control volumes of the primal mesh $\mathcal{M}$ by K and L , and with every primal cell we associate an internal point, e.g., $x_K \in K$. Different choices are possible, which give rise to different versions of the same scheme, such as the barycenters or the arithmetic average of the position vector of cell vertices (also called “isobarycenters”). For the results shown here, we used the second choice, but apparently there is no significant difference between the two choices mentioned above as far as accuracy and convergence behavior are concerned. The vertices, the edges, and the faces of mesh $\mathcal{M}$ are denoted by x_A , E and F , respectively. Also, we denote the

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midpoint of E by x_E and the barycenter of F by x_F . We associate a degree of freedom (the scheme unknowns) with each one of these points; hence, the unknown scalar variable takes the form:

$$u^{\mathcal{T}} = ((u_K)_{K \in \mathcal{M}}, (u_A)_{A \in \mathcal{N}}, (u_E)_{E \in \mathcal{E}}, (u_F)_{F \in \mathcal{F}}).$$

We denote the collections of the boundary items (vertices, edges and faces) by $\partial \mathcal{N}$, $\partial \mathcal{F} \mathcal{E}$ and we introduce the set of boundary cells $\partial \mathcal{M}$ which is composed by the boundary faces here considered as degenerated control volumes. Dirichlet boundary conditions are easily introduced into the scheme through the set of boundary data

$$\delta u^{\mathcal{T}} = ((u_K)_{x_K \in \partial \mathcal{M}}, (u_A)_{x_A \in \partial \mathcal{N}}, (u_E)_{x_E \in \partial \mathcal{F} \mathcal{E}}, (u_F)_{x_F \in \partial \mathcal{F} \mathcal{E}}).$$

The scalar solution field u is approximated by the degrees of freedom $(u^{\mathcal{T}}, \delta u^{\mathcal{T}})$.

The gradient formula is given on each diamond cell $D \in \mathcal{D}$, which is the convex hull of the points K, L, x_A, x_B, x_F, x_E , by

$$\nabla_{\delta u}^D u^{\mathcal{T}} = \frac{1}{3|D|} ((u_L - u_K)N_{KL} + (u_B - u_A)N_{AB} + (u_F - u_E)N_{EF}) \quad (1)$$

using the normal vectors $N_{KL} = \frac{1}{2}(x_B - x_A) \times (x_F - x_E)$, $N_{AB} = \frac{1}{2}(x_F - x_E) \times (x_L - x_K)$ and $N_{EF} = \frac{1}{2}(x_L - x_K) \times (x_B - x_A)$. Gradient formula (1) allows us to define the numerical flux through each interface of the control volumes of the three meshes $\mathcal{M}$, $\mathcal{N}$ and $\mathcal{F} \mathcal{E}$. Let $\mathbf{Q}$ be the linear space of piecewise constant vector fields defined on the mesh of diamonds $\mathcal{D}$ and X be the linear space of triples of piecewise constant scalar fields defined on the three meshes $\mathcal{M}$, $\mathcal{N}$ and $\mathcal{F} \mathcal{E}$. Three finite volume schemes are written by using a discrete divergence operator that maps each vector field in $\mathbf{Q}$ to a triple of scalar functions in X . Formally, we introduce the operator

$$\text{div}^{\mathcal{T}} : \xi = (\xi_D)_{D \in \mathcal{D}} \in \mathbf{Q} \mapsto (\text{div}^{\mathcal{M}} \xi, \text{div}^{\mathcal{N}} \xi, \text{div}^{\mathcal{F} \mathcal{E}} \xi) \in X$$

whose components

$$\text{div}^{\mathcal{M}} \xi = (\text{div}_K \xi)_K, \text{div}^{\mathcal{N}} \xi = (\text{div}_A \xi)_A \text{ and } \text{div}^{\mathcal{F} \mathcal{E}} \xi = \{(\text{div}_E \xi)_E, (\text{div}_F \xi)_F\}$$

are given by

$$|K| \text{div}_K \xi = \sum_{D \in \mathcal{D}_K} \xi_D \cdot N_{KL}, \quad |A| \text{div}_A \xi = \sum_{D \in \mathcal{D}_A} \xi_D \cdot N_{AB}, \quad (2)$$

$$|E| \text{div}_E \xi = \sum_{D \in \mathcal{D}_E} \xi_D \cdot N_{EF}, \quad |F| \text{div}_F \xi = \sum_{D \in \mathcal{D}_F} \xi_D \cdot (-N_{EF}). \quad (3)$$

In the previous statements, the symbols D_K, D_A, D_E, D_F refer to the diamond cells which overlap the cells labeled by the corresponding subscripted indices K, A, E , and L .

Since each of the $\text{div}_C \xi$ approximates $\frac{1}{|C|} \int_C \text{div} \xi$ (for $C = K, A, E, F$), the right hand side of the discrete problem is given by the piecewise constant projection of

the function f onto the space X , $\pi^{\mathcal{T}} f = \{(f_K)_{K \in \mathcal{M}}, (f_A)_{A \in \mathcal{N}}, (f_E, f_F)_{E \in \mathcal{E}, F \in \mathcal{F}}\}$ with $f_C = \frac{1}{|C|} \int_C f(x) dx$ for any cell $C = K \in \mathcal{M}$ or $A \in \mathcal{N}$ or F or $E \in \mathcal{F}$.

The CeVeFE-DDFV scheme reads:

$$-\operatorname{div}^{\mathcal{T}}(\mathbf{K}_D \nabla_{\delta u}^D u^{\mathcal{T}}) = \pi^{\mathcal{T}} f, \quad (4)$$

where $\mathbf{K}_D = \frac{1}{|D|} \int_D \mathbf{K}(x) dx$ is a piecewise constant tensor field on the mesh of the diamond cells. The scheme in (4) originates a symmetric and positive-definite linear system of equations (see [1] for a thorough discussion of the other properties). The case of the discontinuous permeability tensor of test 5 deserves a special treatment that is thoroughly discussed in [2].

Mesure on the error

To put the discrete and the exact solutions “at the same level”, we use the projection $\pi^{\mathcal{T}} u_e$ of the exact solution and the associated discrete gradient reconstruction $\nabla^{\mathcal{T}} \pi^{\mathcal{T}} u_e$. Approximation errors are evaluated through the following norms:

$$\begin{aligned} \text{erl2} &= \|e^{\mathcal{T}}\|_{L^2} / \|\pi^{\mathcal{T}} u_e\|_{L^2} \text{ with } \|e^{\mathcal{T}}\|_{L^2}^2 = \frac{1}{3} \sum_{C \in \mathcal{M} \cup \mathcal{N} \cup \mathcal{F} \cup \mathcal{E}} |C| |e_C|^2 \\ \text{egrad} &= \|\nabla^{\mathcal{T}} e^{\mathcal{T}}\|_{L^2} / \|\nabla^{\mathcal{T}} \pi^{\mathcal{T}} u_e\|_{L^2} \text{ with } \|\nabla^{\mathcal{T}} e^{\mathcal{T}}\|^2 = \sum_{D \in \mathcal{D}} |D| |\nabla^D e^{\mathcal{T}}|^2 \\ \text{ener} &= (\mathbf{K}^{\mathcal{D}} \nabla^{\mathcal{T}} e^{\mathcal{T}}, \nabla^{\mathcal{T}} e^{\mathcal{T}})_{L^2} / (\mathbf{K}^{\mathcal{D}} \nabla^{\mathcal{T}} \pi^{\mathcal{T}} u_e, \nabla^{\mathcal{T}} \pi^{\mathcal{T}} u_e)_{L^2} \\ &\quad \text{with } (\mathbf{K}^{\mathcal{D}} \nabla^{\mathcal{T}} e^{\mathcal{T}}, \nabla^{\mathcal{T}} e^{\mathcal{T}})_{L^2} = \sum_{D \in \mathcal{D}} |D| (\mathbf{K}_D \nabla^D e^{\mathcal{T}}, \nabla^D e^{\mathcal{T}}) \end{aligned}$$

In the case of the discontinuous tensor of test 5, the diamond cell D is divided in two subdiamond cells, namely, D_K and D_L . The gradient $\nabla^D u$ is constant on D_K (respectively, D_L) with value $\nabla_K^D u$ (respectively, $\nabla_L^D u$). The quantities $\|\nabla^{\mathcal{T}} e^{\mathcal{T}}\|_{L^2}^2$ and $(\mathbf{K}^{\mathcal{D}} \nabla^{\mathcal{T}} e^{\mathcal{T}}, \nabla^{\mathcal{T}} e^{\mathcal{T}})_{L^2}$ become

$$\|\nabla^{\mathcal{T}} e^{\mathcal{T}}\|_{L^2}^2 = \sum_{D \in \mathcal{D}} (|D_K| |\nabla_{D_K} e^{\mathcal{T}}|^2 + |D_L| |\nabla_{D_L} e^{\mathcal{T}}|^2)$$

and

$$(\mathbf{K}^{\mathcal{D}} \nabla^{\mathcal{T}} e^{\mathcal{T}}, \nabla^{\mathcal{T}} e^{\mathcal{T}})_{L^2} = \sum_{D \in \mathcal{D}} (|D_K| (\mathbf{K}_{D_K} \nabla_{D_K} e^{\mathcal{T}}, \nabla_{D_K} e^{\mathcal{T}}) + |D_L| (\mathbf{K}_{D_L} \nabla_{D_L} e^{\mathcal{T}}, \nabla_{D_L} e^{\mathcal{T}})).$$

2 Numerical results

The following results were obtained by using a BiCG-stab solver with ILU(0) preconditioner (routine MI26 of HSL implementation).

- **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	7777	100569	6.09E-03	1.05E-02	1.988	1.980	1.790
2	15495	208527	7.48E-03	9.35E-03	1.995	1.994	1.793
3	31139	431667	3.19E-03	5.93E-03	1.993	1.993	1.795
4	62419	885735	1.48E-03	2.98E-03	1.996	1.996	1.796
5	125993	1823199	1.56E-03	2.28E-03	2.000	1.999	1.797
6	254657	3746829	1.93E-03	2.70E-03	1.999	1.998	1.798

i	nu	erl2	ratl2	ergrad	ratioegrad	ener	ratioener
1	7777	0.228E-02	-	0.562E-01	-	0.528E-01	-
2	15495	0.147E-02	1.904	0.441E-01	1.051	0.415E-01	1.054
3	31139	0.916E-03	2.036	0.349E-01	1.011	0.327E-01	1.021
4	62419	0.573E-03	2.025	0.276E-01	1.006	0.258E-01	1.022
5	125993	0.374E-03	1.819	0.219E-01	0.994	0.206E-01	0.969
6	254657	0.231E-03	2.067	0.174E-01	0.983	0.163E-01	0.990

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

i	nu	nmat	umin	uemin	umax	uemax	normg
1	345	4559	7.93E-02	1.51E-01	1.875	1.844	1.719
2	933	12811	4.79E-02	4.74E-02	1.989	1.982	1.785
3	2075	29291	5.46E-02	5.64E-02	1.987	1.978	1.794
4	3963	56947	3.25E-02	3.23E-02	2.000	1.996	1.795
5	6909	101229	1.28E-02	3.17E-02	2.000	1.996	1.797

i	nu	erl2	ratl2	ergrad	ratioegrad	ener	ratioener
1	345	0.274E-01	-	0.179E+00	-	0.162E+00	-
2	933	0.223E-01	0.622	0.149E+00	0.556	0.139E+00	0.458
3	2075	0.119E-01	2.364	0.102E+00	1.409	0.964E-01	1.373
4	3963	0.819E-02	1.724	0.835E-01	0.933	0.782E-01	0.972
5	6909	0.599E-02	1.694	0.691E-01	1.021	0.655E-01	0.953

- **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	3375	49071	5.67E-02	3.43E-02	1.940	1.974	1.767
2	29791	455895	9.19E-03	7.33E-03	1.988	1.991	1.782
3	250047	3916359	2.42E-03	1.59E-03	1.999	1.998	1.793
4	2048383	32446751	6.52E-04	6.17E-04	2.000	1.999	1.797

i	nu	erl2	ratl2	ergrad	ratioegrad	ener	ratioener
1	3375	0.287E-01	-	0.481E+00	-	0.589E+00	-
2	29791	0.113E-01	1.289	0.218E+00	1.088	0.233E+00	1.277
3	250047	0.330E-02	1.730	0.904E-01	1.243	0.953E-01	1.260
4	2048383	0.859E-03	1.922	0.395E-01	1.180	0.422E-01	1.161

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

i	nu	nmat	umin	uemin	umax	uemax	normg
1	239	2871	8.58E-02	8.40E-02	1.903	1.916	1.795
2	2543	34927	2.90E-02	2.13E-02	1.971	1.979	1.804
3	23135	336735	4.68E-03	5.35E-03	1.995	1.995	1.800
4	196799	2943487	1.69E-03	1.34E-03	1.998	1.999	1.799
5	1622399	24588351	2.88E-04	3.35E-04	2.000	2.000	1.799

i	nu	erl2	ratl2	ergrad	ratioegrad	ener	ratioener
1	239	0.307E-01	-	0.141E+00	-	0.139E+00	-
2	2543	0.120E-01	1.190	0.104E+00	0.384	0.101E+00	0.405
3	23135	0.323E-02	1.786	0.571E-01	0.814	0.550E-01	0.827
4	196799	0.830E-03	1.905	0.298E-01	0.909	0.285E-01	0.920
5	1622399	0.210E-03	1.955	0.154E-01	0.937	0.147E-01	0.945

- **Test 2 Heterogeneous anisotropy**,
 $u(x, y, z) = x^3 y^2 z + x \sin(2\pi x z) \sin(2\pi x y) \sin(2\pi z)$, $\min = -0.862$, $\max = 1.0487$,
Prism meshes

i	nu	nmat	umin	uemin	umax	uemax	normg
1	12179	188089	-8.55E-01	-8.46E-01	1.014	1.009	1.693
2	96759	1545215	-8.55E-01	-8.57E-01	1.026	1.031	1.706
3	325739	5259545	-8.61E-01	-8.59E-01	1.037	1.035	1.708
4	771119	12518433	-8.60E-01	-8.60E-01	1.040	1.041	1.709

i	nu	erl2	ratl2	ergrad	ratioegrad	ener	ratioener
1	12179	0.392E-01	-	0.811E-01	-	0.803E-01	-
2	96759	0.109E-01	1.854	0.392E-01	1.054	0.397E-01	1.019
3	325739	0.502E-02	1.917	0.256E-01	1.051	0.261E-01	1.040
4	771119	0.287E-02	1.942	0.190E-01	1.039	0.194E-01	1.034

- **Test 3 Flow on random meshes, $u(x, y, z) = \sin(\pi x) \sin(\pi y) \sin(\pi z)$,
min = 0, max = 1, Random meshes**

i	nu	nmat	umin	uemin	umax	uemax	normg
1	343	4447	-4.25E+01	-9.78E-01	49.169	0.931	38.139
2	3375	49855	-2.22E+01	-9.94E-01	21.970	0.982	21.514
3	29791	466111	-6.96E+00	-9.95E-01	7.051	0.993	12.536
4	250047	4019647	-2.67E+00	-9.98E-01	2.725	0.998	7.541

i	nu	erl2	ratl2	ergrad	ratioegrad	ener	ratioener
1	343	0.147E+03	-	0.238E+02	-	0.162E+01	-
2	3375	0.956E+01	3.589	0.121E+02	0.892	0.888E+00	0.787
3	29791	0.681E+00	3.640	0.632E+01	0.891	0.459E+00	0.909
4	250047	0.447E-01	3.840	0.314E+01	0.988	0.229E+00	0.979

- **Test 4 Flow around a well, Well meshes, min = 0, max = 5.415**

i	nu	nmat	umin	uemin	umax	uemax	normg
1	5868	86728	3.83E-01	4.13E-01	5.317	5.317	1596.292
2	15776	243104	2.37E-01	2.43E-01	5.328	5.328	1611.158
3	36846	580244	1.54E-01	1.54E-01	5.329	5.329	1617.452
4	84546	1350382	1.17E-01	1.18E-01	5.330	5.330	1620.143
5	177590	2860258	8.96E-02	8.98E-02	5.339	5.339	1621.406
6	329236	5329338	7.22E-02	7.23E-02	5.345	5.345	1622.053
7	580190	9422104	5.66E-02	5.64E-02	5.361	5.361	1622.472

i	nu	erl2	ratl2	ergrad	ratioegrad	ener	ratioener
1	5868	0.141E-04	-	0.128E+00	-	0.116E+00	-
2	15776	0.476E-05	3.290	0.877E-01	1.144	0.781E-01	1.212
3	36846	0.208E-05	2.924	0.610E-01	1.283	0.542E-01	1.287
4	84546	0.141E-05	1.411	0.466E-01	0.975	0.408E-01	1.033
5	177590	0.914E-06	1.747	0.362E-01	1.021	0.316E-01	1.023
6	329236	0.609E-06	1.976	0.293E-01	1.026	0.258E-01	0.998
7	580190	0.422E-06	1.941	0.244E-01	0.964	0.214E-01	0.971

- **Test 5 Discontinuous permeability**, $u(x, y, z) = \sin(\pi x) \sin(\pi y) \sin(\pi z)$,
min = 0, max = 1, **Locally refined meshes**

i	nu	nmat	umin	uemin	umax	uemax	normg
1	131	1017	-6.34E+01	-1.00E+02	64.462	100.000	85.763
2	1215	8303	-3.10E+02	-1.00E+02	309.886	100.000	192.379
3	10463	65007	-1.34E+02	-1.00E+02	134.323	100.000	139.345
4	86847	509567	-1.09E+02	-1.00E+02	109.373	100.000	114.251
5	707711	4024287	-1.02E+02	-1.00E+02	102.394	100.000	104.279

i	nu	erl2	ratl2	ergrad	ratiograd	ener	ratioener
1	131	0.218E+01	-	0.450E+00	-	0.406E+00	-
2	1215	0.193E+01	0.159	0.187E+01	-1.917	0.623E+00	-0.578
3	10463	0.862E-01	4.334	0.828E+00	1.134	0.297E+00	1.033
4	86847	0.517E-02	3.989	0.407E+00	1.006	0.147E+00	0.995
5	707711	0.326E-03	3.953	0.203E+00	0.994	0.734E-01	0.994

3 Comments

This finite volume method assigns one degree of freedom to any mesh item (cells, faces, edges, and vertices). For this reason, the scheme has a large number of degrees of freedom if compared to other finite volume methods or similar discretization techniques (such as mimetic finite differences). Nonetheless, the method was proved very effective both for two and three dimensional problems with strong anisotropic coefficients and using meshes with strongly distorted cells. Among the other advantages offered by the method, we mention the coercivity of the method that eases the convergence analysis and the fact that this finite volume method generally shows second order of accuracy in all numerical experiments where the exact solution is sufficiently regular. The results shown in the tables of the previous section confirm this general behavior.

All linear systems were solved efficiently by standard preconditioned Krylov methods as BiCG-stab or GMRES. Direct solvers for general asymmetric systems (UMFPACK) can also be used, but they normally require a huge memory storage, in particular for the biggest problems. In Table 1-2, we see an example of the performance of the different solvers offered by the benchmark site when solving Test 1 on the checkerboard meshes $8 \times 8 \times 8$ and $16 \times 16 \times 16$. The comparison reveals that PETSc implementation of the CG solver is the fastest one, in particular, when combined with the diagonal preconditioner (Jacobi). A good performance in terms of CPU costs is also provided by the ISTL-BiCGstab implementation using Jacobi or ILU(0) preconditioners. CPU times are usually smaller than those obtained by using the direct solver UMFPACK, which is also available in the benchmark site.

For example, in the case of $8 \times 8 \times 8$ -size mesh we note that UMFPACK requires a CPU time of 3.180 seconds.

solver	precond	CPU time	# iters	Rel. resid.
PETSc-CG	Jacobi	0.209	202	6.368e-11
PETSc-CG	none	0.243	242	1.715e-10
ISTL-BiCGstab	ILU(0)	0.404	53	6.832e-11
ISTL-BiCGstab	none	0.563	167	3.656e-11
ISTL-BiCGstab	Jacobi	0.680	120	4.415e-11
ISTL-GMRES	ILU(0)	0.683	152	4.241e-11

Table 1 CeVeFe-DDFV method, test 1 using checkerboard mesh, grid resolution $8 \times 8 \times 8$; CPU times are measured in seconds.

solver	precond	CPU time	# iters	Rel. resid.
PETSc-CG	Jacobi	3.946	369	4.248e-11
PETSc-CG	none	4.989	471	8.038e-11
ISTL-CG	ILU(0)	5.540	166	4.041e-11
ISTL-CG	none	7.319	471	8.038e-11
ISTL-BiCGstab	ILU(0)	8.681	107	3.873e-11
ISTL-CG	Jacobi	10.989	368	4.281e-11

Table 2 CeVeFe-DDFV method, test 1 using checkerboard mesh, grid resolution $16 \times 16 \times 16$; CPU times are measured in seconds.

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