# Benchmark 3D: The Cell-Centered Finite Volume Method Using Least Squares Vertex Reconstruction ("Diamond Scheme")

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## 1 Presentation of the scheme

We consider, for this contribution, the cell-centered finite volume method based on least squares vertex reconstruction. This method, which is also popularly known as *"the diamond scheme"*, was originally presented for the advection-diffusion equation in two-dimensions and then extended in 3-D. The discretization of the diffusive term in 2-D and 3-D is found in in [1, 3–5]. The scalar solution of the diffusion problem $u$ is numerically approximated by a piecewise constant function $u_T$ on the cells $K$ of mesh $T$. The numerical approximation $u_T$ is defined as $u_T(x) = \sum_{K\in T} u_K \chi_K(x)$ ($\chi_K(x)$ being the characteristic function of cell $K$) through the values $(u_K)_{K\in T}$. To define the numerical diffusive flux through the interface $f$ of the mesh, a polyhedral cell is built around this interface. This polyhedral cell, which has a quadrilateral shape in two dimensions, is named after its shape as *"diamond cell"*, which also motivates the name of the method. Specifically, let $x_K \in K$ be the center of gravity of the cell $K$ of mesh $T$. The diamond cell $D$ associated to the interface $f$ between two cells $K$ and $L$ in $T$ is the convex hull $D = \text{hull}(f, x_K, x_L)$. If $f$ is a boundary face, thus defined by $f = \partial K \cap \partial\Omega$ where $\partial\Omega$ is the boundary of the computational domain $\Omega$, then the diamond cell associated to $f$ is the convex hull $D = \text{hull}(f, x_K)$.

The numerical diffusive flux is built by using a constant approximation of the solution gradient on each diamond cell. Let $(x_1, x_2, \ldots x_m)$ denote the vertices of face $f$, $x_K$ and $x_L$ the centers of gravity of the cells $K$ and $L$ that share this face, and $D$ the convex hull of these points. For any function $u \in H^1(D)$, the Green-Gauss formula yields the relation $\int_D \nabla u(x)dx = \int_{\partial D} u(x)n(x)d\sigma(x)$, where $n$ is

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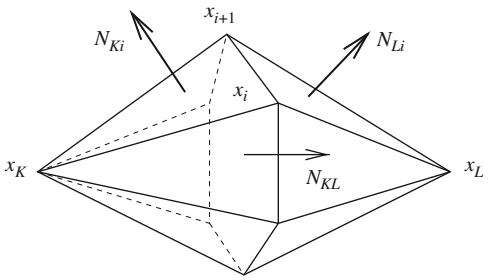


**Fig. 1** Geometry of the *diamond* cell

the unit vector orthogonal to $\partial D$ and pointing out of $D$. If the restriction of $u$ to the face $f$ of $\partial D$ is an affine function, the boundary integral only depends on the values of $u$ at the vertices of $D$. In this case, the Green-Gauss divergence theorem yields

$$\frac{1}{|D|}\int_D \nabla u(x)dx = \frac{1}{|D|}\int_{\partial D} u(x)n(x)dx = \frac{1}{|D|}\sum_{f\in\partial D}\int_f u(x)n(x)dx$$

$$= \frac{1}{3|D|}\sum_{i=1}^{m}\big(N_{Ki}(u(x_i)+u(x_{i+1})+u(x_K)) + N_{Li}(u(x_i)+u(x_{i+1})+u(x_L))\big)$$

$$= \frac{1}{3|D|}\Big(\big(u(x_L)-u(x_K)\big)N_{KL} + \sum_{i=1}^{m} u(x_i)N_i\Big),$$

where $N_{Ki}$ and $N_{Li}$ are the vectors orthogonal to the triangular facets $\mathrm{hull}(x_K, x_i, x_{i+1})$ and $\mathrm{hull}(x_L, x_i, x_{i+1})$, respectively, and having lengths equal to the measure of the facets; specifically, $N_{Ki} = \frac{1}{2}(x_i - x_K)\times(x_{i+1} - x_K)$ and $N_{Li} = -\frac{1}{2}(x_i - x_L)\times(x_{i+1} - x_L)$, see Fig. 1. The vectors $N_{KL}$ and $N_i$ actually used during the computations are

$$N_{KL} = \sum_{i=1}^{m} N_{Li} = -\sum_{i=1}^{m} N_{Ki} \quad \text{and} \quad N_i = N_{Ki} + N_{Li} + N_{Ki-1} + N_{Li-1}.$$

To derive the gradient formula, we consider the right-hand side of the above equality with the unknown $u_K$ and $u_L$ replacing $u(x_K)$ and $u(x_L)$ and some values $u_i$ replacing the values $u(x_i)$. These values, $u_1, u_2, \ldots u_m$, are linearly interpolated from the values $(u_K)_{K\in T}$ as follows. For any vertex $x_i$ of the mesh $T$, we consider $u_i = \sum_{K\in T_i}\omega_{iK}u_K$ where $T_i = \{K : x_i \in K\}$ denotes the subset of the mesh cells which share the vertex $x_i$. The interpolation weights $\omega_{iK}$ are assumed to verify the consistency relations [4]:

$$\sum_{K\in T_i}\omega_{iK} = 1 \quad \text{and} \quad \sum_{K\in T_i}\omega_{iK}(x_i - x_K) = 0.$$

The interpolation weights $\omega_{iK}$ are obtained by solving the reconstruction problem that approximates the cell-averaged data set $\{(x_K, u_K)$ for $K \in T_i\}$ by the affine function

$$\tilde{u}_i(x) = \alpha + \beta \cdot (x - x_i) \quad \text{for } x \in \mathcal{V}_i$$

on the co-volume $\mathcal{V}_i = \bigcup_{K \in T_i} K$ and in a least square sense, cf. [2, 4]. The reconstructed value at vertex $x_i$ is now given by taking $u_i = \tilde{u}_i(x_i) = \alpha$. The coefficients $(\alpha, \beta)^T$ are the minimizers of the least squares functional

$$\mathcal{J}(\alpha, \beta^T) = \sum_{K : x_i \in K} \big(\alpha + \beta \cdot (x - x_i) - u_K\big)^2.$$

Imposing the zero gradient condition, i.e., $\nabla_{\alpha,\beta} \mathcal{J}(\alpha, \beta^T) = 0$, yields a linear system for the coefficients $(\alpha, \beta)$, whose solution returns the interpolation weights. The values $u_i$ at the vertices $x_i \in \partial\Omega$ on the Dirichlet boundary are constrained to the boundary data, for instance $u_i = 0$ for a homogeneous condition. Other kinds of boundary conditions, e.g., Neumann or Robin, can be taken into account by extending to the 3-D case the technique investigated in [2]. Finally, the scheme reads as

$$\forall K \in T, \quad -\sum_{f \subset \partial K} \Lambda_f \nabla_D u_T \cdot N_{KL} = f_K |K| := \int_K f(x) dx,$$

where $\Lambda_f$ is an arithmetic average of the diffusion tensor $\Lambda$ over the diamond cell located around face $f$ and $N_{KL}$ is exactly the normal from above.

## 2 Numerical 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 |
|---|---|---|---|---|---|---|---|
| 0 | 215 | 6985 | 3.02E-02 | 3.15E-02 | 1.949 | 1.948 | 1.627 |
| 1 | 2003 | 107331 | 2.03E-02 | 1.13E-02 | 1.989 | 1.995 | 1.730 |
| 2 | 3898 | 227618 | 6.84E-03 | 4.21E-03 | 1.989 | 1.990 | 1.750 |
| 3 | 7711 | 476645 | 9.13E-03 | 8.18E-03 | 1.994 | 1.995 | 1.767 |
| 4 | 15266 | 994892 | 5.52E-03 | 4.10E-03 | 1.997 | 1.997 | 1.776 |
| 5 | 30480 | 2072944 | 1.49E-03 | 2.57E-04 | 1.997 | 1.999 | 1.784 |
| 6 | 61052 | 4292073 | 1.83E-03 | 1.20E-03 | 1.997 | 1.998 | 1.789 |

| i | nu | erl2 | ratiol2 | ergrad | ratiograd | ener | ratioener |
|---|---|---|---|---|---|---|---|
| 0 | 215 | 3.750E-02 | - | 3.503E-01 | - | 2.636E-01 | - |
| 1 | 2003 | 9.173E-03 | 1.892 | 1.568E-01 | 1.081 | 1.071E-01 | 1.210 |
| 2 | 3898 | 5.897E-03 | 1.991 | 1.215E-01 | 1.149 | 8.159E-02 | 1.225 |
| 3 | 7711 | 3.551E-03 | 2.230 | 9.410E-02 | 1.122 | 6.016E-02 | 1.339 |
| 4 | 15266 | 2.255E-03 | 1.994 | 7.387E-02 | 1.063 | 4.648E-02 | 1.132 |
| 5 | 30480 | 1.412E-03 | 2.032 | 5.768E-02 | 1.073 | 3.565E-02 | 1.152 |
| 6 | 61052 | 8.882E-04 | 2.001 | 4.502E-02 | 1.070 | 2.733E-02 | 1.147 |

Name of the solver: BiCG-stab with Jacobi preconditioner (in-house implementation).

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

| i | nu | nmat | umin | uemin | umax | uemax | normg |
|---|---|---|---|---|---|---|---|
| 1 | 29 | 257 | 8.51E-02 | -6.18E+00 | 1.870 | 7.968 | 20.435 |
| 2 | 66 | 660 | 1.43E-01 | 2.06E-01 | 1.854 | 1.846 | 1.887 |
| 3 | 130 | 1410 | 3.85E-02 | 7.00E-03 | 1.925 | 1.941 | 1.855 |
| 4 | 228 | 2620 | 1.74E-02 | 2.37E-02 | 1.914 | 1.920 | 2.067 |
| 5 | 356 | 4424 | 2.84E-03 | -2.18E+00 | 1.979 | 3.546 | 3.274 |

| i | nu | erl2 | ratiol2 | ergrad | ratiograd | ener | ratioener |
|---|---|---|---|---|---|---|---|
| 1 | 29 | 2.639E+00 | - | 3.631E+01 | - | 9.728E+00 | - |
| 2 | 66 | 9.077E-02 | 12.292 | 9.457E-01 | 13.307 | 3.751E-01 | 11.876 |
| 3 | 130 | 5.508E-02 | 2.210 | 7.434E-01 | 1.065 | 3.055E-01 | 0.907 |
| 4 | 228 | 6.650E-02 | -1.006 | 1.163E+00 | -2.391 | 3.224E-01 | -0.287 |
| 5 | 356 | 3.674E-01 | -11.507 | 5.071E+00 | -9.912 | 1.287E+00 | -9.321 |

Name of the solver: BiCG-stab with Jacobi preconditioner (in-house implementation).

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

| i | nu | nmat | umin | uemin | umax | uemax | normg |
|---|---|---|---|---|---|---|---|
| 1 | 512 | 10648 | 3.03E-02 | 8.74E-02 | 1.958 | 1.916 | 1.768 |
| 2 | 4096 | 97336 | 1.06E-02 | 3.00E-02 | 1.993 | 1.973 | 1.700 |
| 3 | 32768 | 830584 | 1.75E-03 | 5.87E-03 | 1.997 | 1.991 | 1.726 |
| 4 | 262144 | 6859000 | 7.14E-04 | 9.88E-04 | 1.999 | 1.998 | 1.765 |

| i | nu | erl2 | ratiol2 | ergrad | ratiograd | ener | ratioener |
|---|---|---|---|---|---|---|---|
| 1 | 512 | 6.846E-02 | - | 6.798E-01 | - | 4.901E-01 | - |
| 2 | 4096 | 4.715E-02 | 0.537 | 3.403E-01 | 0.998 | 2.715E-01 | 0.851 |
| 3 | 32768 | 2.866E-02 | 0.718 | 1.831E-01 | 0.894 | 1.532E-01 | 0.825 |
| 4 | 262144 | 1.315E-02 | 1.123 | 8.289E-02 | 1.143 | 6.942E-02 | 1.142 |

Name of the solver: BiCG-stab with Jacobi preconditioner (in-house implementation).

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

| i | nu | nmat | umin | uemin | umax | uemax | normg |
|---|---|---|---|---|---|---|---|
| 1 | 36 | 424 | 1.54E-01 | 1.33E-01 | 1.846 | 1.833 | 1.588 |
| 2 | 288 | 4528 | 4.01E-02 | 3.47E-02 | 1.960 | 1.958 | 1.721 |
| 3 | 2304 | 41896 | 1.01E-02 | 8.74E-03 | 1.990 | 1.990 | 1.773 |
| 4 | 18432 | 360280 | 2.54E-03 | 1.98E-03 | 1.997 | 1.998 | 1.791 |
| 5 | 147456 | 2987704 | 6.36E-04 | 5.26E-04 | 1.999 | 1.999 | 1.796 |

| i | nu | erl2 | ratiol2 | ergrad | ratiograd | ener | ratioener |
|---|---|---|---|---|---|---|---|
| 1 | 36 | 1.356E-01 | - | 2.488E-01 | - | 3.406E-01 | - |
| 2 | 288 | 4.427E-02 | 1.615 | 1.471E-01 | 0.758 | 1.346E-01 | 1.339 |
| 3 | 2304 | 1.191E-02 | 1.894 | 7.031E-02 | 1.065 | 4.678E-02 | 1.524 |
| 4 | 18432 | 3.112E-03 | 1.936 | 3.410E-02 | 1.043 | 1.687E-02 | 1.471 |
| 5 | 147456 | 7.976E-04 | 1.964 | 1.695E-02 | 1.008 | 7.003E-03 | 1.268 |

Name of the solver: BiCG-stab with Jacobi preconditioner (in-house implementation).

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

| i | nu | nmat | umin | uemin | umax | uemax | normg |
|---|---|---|---|---|---|---|---|
| 1 | 1210 | 21308 | -8.42E-01 | -8.57E-01 | 0.978 | 0.977 | 1.481 |
| 2 | 8820 | 169418 | -8.38E-01 | -8.41E-01 | 1.010 | 1.011 | 1.638 |
| 3 | 28830 | 570328 | -8.58E-01 | -8.60E-01 | 1.032 | 1.033 | 1.676 |
| 4 | 67240 | 1350038 | -8.57E-01 | -8.58E-01 | 1.033 | 1.034 | 1.690 |

| i | nu | erl2 | ratiol2 | ergrad | ratiograd | ener | ratioener |
|---|---|---|---|---|---|---|---|
| 1 | 1210 | 9.551E-02 | - | 2.356E-01 | - | 2.404E-01 | - |
| 2 | 8820 | 2.403E-02 | 2.084 | 8.174E-02 | 1.598 | 7.974E-02 | 1.666 |
| 3 | 28830 | 1.067E-02 | 2.057 | 4.167E-02 | 1.706 | 3.947E-02 | 1.781 |
| 4 | 67240 | 6.013E-03 | 2.030 | 2.562E-02 | 1.722 | 2.371E-02 | 1.805 |

Name of the solver: BiCG-stab with Jacobi preconditioner (in-house implementation).

• **Test 3 Flow on random meshes,** $u(x, y, z) = \sin(2\pi x) \sin(2\pi y) \sin(2\pi z)$**,** $\min = 0$, $\max = 1$**, Random meshes**

| i | nu | nmat | umin | uemin | umax | uemax | normg |
|---|---|---|---|---|---|---|---|
| 1 | 64 | 1000 | -7.56E-01 | -7.11E-01 | 0.711 | 0.525 | 1.650 |
| 2 | 512 | 10648 | -9.39E-01 | -8.32E-01 | 0.926 | 0.933 | 2.674 |
| 3 | 4096 | 97336 | -9.86E-01 | -9.77E-01 | 0.982 | 0.978 | 3.330 |
| 4 | 32768 | 830584 | -9.96E-01 | -9.92E-01 | 0.996 | 0.990 | 3.527 |

| i | nu | erl2 | ratiol2 | ergrad | ratiograd | ener | ratioener |
|---|---|---|---|---|---|---|---|
| 1 | 64 | 5.548E-01 | - | 7.060E-01 | - | 7.651E-01 | - |
| 2 | 512 | 1.427E-01 | 1.958 | 3.067E-01 | 1.202 | 3.264E-01 | 1.229 |
| 3 | 4096 | 2.967E-02 | 2.266 | 9.532E-02 | 1.685 | 9.569E-02 | 1.770 |
| 4 | 32768 | 7.166E-03 | 2.049 | 3.253E-02 | 1.551 | 2.529E-02 | 1.919 |

Name of the solver: BiCG-stab with Jacobi preconditioner (in-house implementation).

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

| i | nu | nmat | umin | uemin | umax | uemax | normg |
|---|---|---|---|---|---|---|---|
| 1 | 890 | 18876 | 4.57E-01 | 5.26E-01 | 5.317 | 5.318 | 1573.020 |
| 2 | 2232 | 51800 | 2.61E-01 | 2.89E-01 | 5.329 | 5.329 | 1600.780 |
| 3 | 5016 | 121584 | 1.62E-01 | 1.73E-01 | 5.329 | 5.329 | 1613.840 |
| 4 | 11220 | 280868 | 1.23E-01 | 1.29E-01 | 5.330 | 5.330 | 1619.520 |
| 5 | 23210 | 592448 | 9.28E-02 | 9.66E-02 | 5.339 | 5.339 | 1620.960 |
| 6 | 42633 | 1100865 | 7.42E-02 | 7.67E-02 | 5.345 | 5.345 | 1621.200 |
| 7 | 74679 | 1942619 | 5.75E-02 | 5.91E-02 | 5.361 | 5.361 | 1621.930 |

| i | nu | erl2 | ratiol2 | ergrad | ratiograd | ener | ratioener |
|---|---|---|---|---|---|---|---|
| 1 | 890 | 9.562E-03 | - | 8.767E-02 | - | 5.372E-02 | - |
| 2 | 2232 | 3.699E-03 | 3.098 | 3.903E-02 | 2.640 | 2.305E-02 | 2.761 |
| 3 | 5016 | 1.676E-03 | 2.932 | 1.916E-02 | 2.636 | 1.104E-02 | 2.727 |
| 4 | 11220 | 1.190E-03 | 1.275 | 1.270E-02 | 1.531 | 7.205E-03 | 1.589 |
| 5 | 23210 | 7.545E-04 | 1.882 | 8.919E-03 | 1.458 | 5.053E-03 | 1.463 |
| 6 | 42633 | 4.601E-04 | 2.439 | 6.148E-03 | 1.835 | 3.522E-03 | 1.781 |
| 7 | 74679 | 3.402E-04 | 1.616 | 5.400E-03 | 0.693 | 3.174E-03 | 0.556 |

Name of the solver: BiCG-stab with Jacobi preconditioner (in-house implementation).

• **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 | 22 | 252 | -1.00E+02 | -5.24E+01 | 100.000 | 52.359 | 58.097 |
| 2 | 176 | 3220 | -3.54E+01 | -2.62E+01 | 35.355 | 26.180 | 43.055 |
| 3 | 1408 | 31524 | -7.89E+01 | -7.30E+01 | 78.858 | 73.021 | 76.757 |
| 4 | 11264 | 277396 | -9.43E+01 | -9.25E+01 | 94.346 | 92.545 | 92.422 |
| 5 | 90112 | 2324532 | -9.86E+01 | -9.81E+01 | 98.562 | 98.089 | 97.247 |

| i | nu | erl2 | ratiol2 | ergrad | ratiograd | ener | ratioener |
|---|---|---|---|---|---|---|---|
| 1 | 22 | 9.831E-01 | - | 7.196E-01 | - | 3.176E+02 | - |
| 2 | 176 | 5.072E-01 | 0.954 | 7.376E-01 | -0.035 | 8.184E-01 | 8.600 |
| 3 | 1408 | 1.376E-01 | 1.882 | 3.770E-01 | 0.968 | 6.058E-01 | 0.433 |
| 4 | 11264 | 3.347E-02 | 2.039 | 1.874E-01 | 1.008 | 4.685E-01 | 0.370 |
| 5 | 90112 | 9.731E-03 | 1.782 | 1.159E-01 | 0.693 | 3.448E-01 | 0.442 |

Name of the solver: BiCG-stab with Jacobi preconditioner (in-house implementation).

## 3 Comments

This finite volume method is truly cell-centered and, for this reason, it has a relatively small number of degrees of freedom with respect to other finite volume discretizations which introduce face unknowns to approximate the scalar variable. The coercivity was proved only for simple cases (see [3] for details), so very few can be said from a theoretical standpoint about the convergence properties of this scheme and the literature misses a general convergence analysis. Despite this fact, the resulting finite volume method generally show second order of accuracy in all numerical experiments where the exact solution is enough regular and on

**Table 1** LS-FVM method, test 1 using Kershaw mesh with grid resolution 32 × 32 × 32; CPU times are measured in seconds.

| solver | precond | CPU time | # iters | Rel. resid. |
|---|---|---|---|---|
| UMFPACK | none | 28.712 | 0 | 7.287e-15 |
| ISTL-BiCGstab | Jacobi | 36.048 | 2990 | 1.126e-10 |
| ISTL-GMRES | Jacobi | 64.775 | 9186 | 3.931e-10 |
| ISTL-BiCGstab | none | 78.880 | 11417 | 3.431e-10 |
| ISTL-BiCGstab | ILU(4) | 1888.48 | 2 | 1.191e-12 |
| ISTL-GMRES | ILU(4) | 1692.49 | 4 | 9.103e-10 |

"reasonable" meshes. Moreover, it can be easily applied to complex, distorted meshes and anisotropic permeabilities for which it provides a reliable numerical approximation. It is also generally robust even if a locking phenomenon for the convergence has been reported in the literature [6].

The linear system for the cell-centered unknowns that is originated by this scheme on a general polyhedral mesh leads to an *asymmetric sparse matrix*. Therefore, this system can be solved efficiently by standard preconditioned Krylov methods (BiCG-stab or GMRES) or by direct solvers for general asymmetric systems (UMFPACK). An example of a typical behavior is reported in Table 1 for a subset of the combinations solvers and preconditioners available on the benchmark site. The comparison among these results reveals that the BiCG-stab solver using a diagonal Jacobi preconditioner seems to be the more efficient choice in most of the cases. The performance is usually comparable with that offered by the direct solver (UMFPACK), but the memory storage required by this latter may be from 2 to 60 times greater.

## References

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