

Monotone scheme for diffusion type problems with heterogeneous anisotropic tensor on unstructured meshes

Konstantin Lipnikov* Mikhail Shashkov* Daniil Svyatskiy* Yuri Vassilevski‡

* Mathematical Modeling and Analysis Group, Los Alamos National Laboratory, Email: lipnikov@lanl.gov, shashkov@lanl.gov, dasvyat@lanl.gov

‡ Institute of Numerical Mathematics, Email: vasilevs@dodo.inm.ras.ru

Practical requirements for a discretization

- be locally conservative;
- preserve positivity of the differential solution;
- be applicable to unstructured, anisotropic, and severely distorted meshes;
- be applicable to heterogeneous full diffusion tensors;
- result in sparse systems with minimal number of non-zero entries.

Scheme description

Let us consider computational domain Ω and its partition \mathcal{T} into triangles. The diffusion equation in the mixed form is

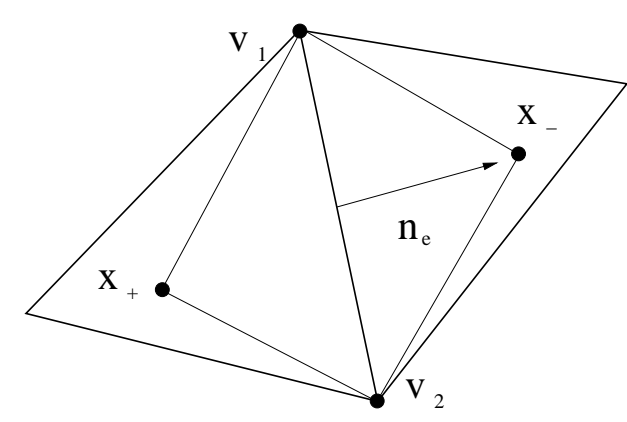
$$\operatorname{div} \mathbf{q} = f \quad \mathbf{q} = -\mathbb{D} \operatorname{grad} C.$$

The conventional approach to the construction of cell-centered finite volume (FV) schemes is based on the cellwise application of the Green formula which results in the equation:

$$\sum_{e \in \partial T} \mathbf{q}_e \cdot \mathbf{n}_e = \int_T f \, dx, \quad \forall T \in \mathcal{T}, \quad \text{where } \mathbf{q}_e = \frac{e}{|e|} \frac{\partial C}{\partial \mathbf{n}_e} \text{ and } |\mathbf{n}_e| = |e|. \quad (1)$$

Cell-centered finite volume discretizations assume that one degree of freedom C_T for C is assigned to each cell T . For each cell T a reference point \mathbf{x}_T is defined (see the definition below) where C is approximated.

Flux definition



Let us consider an internal edge e connecting vertices \mathbf{v}_1 and \mathbf{v}_2 . Points \mathbf{x}_+ and \mathbf{x}_- are reference points which correspond to cells sharing the edge e . The two-point nonlinear flux approximation [C. LePotier, 2005] is derived on the basis of the Green formula and quadrature rules:

$$\mathbf{q}_e \cdot \mathbf{n}_e = A_e^+(C_{v_1}, C_{v_2}) C_{x_+} - A_e^-(C_{v_1}, C_{v_2}) C_{x_-} \quad (2)$$

Interpolation

The values of C at vertices are involved in the flux coefficients in (2). For an approximation of C_{v_1} and C_{v_2} two interpolation techniques may be adopted.

- *linear* (preferable for smooth solutions). Let \mathbf{x}_{T_j} , $j = 1, 2, 3$ be three closest reference points to \mathbf{v}_i , such that triangle $\mathbf{x}_{T_1}\mathbf{x}_{T_2}\mathbf{x}_{T_3}$ contains \mathbf{v}_i . Then

$$C_{v_i} = \sum_{j=1}^3 \lambda_j C_{\mathbf{x}_{T_j}} \quad \text{where } \lambda_j \text{ are the barycentric coordinates of } \mathbf{v}_i.$$

- *inverse distance weighting* [D. Shepard, 1968] (preferable for nonsmooth solutions). The interpolation uses values $C_{\mathbf{x}_T}$ of all triangles sharing \mathbf{v}_i :

$$C_{v_i} = \sum_{T_j \ni \mathbf{v}_i} w_j C_{\mathbf{x}_{T_j}} \quad \text{where } w_j = \frac{|\mathbf{v}_i - \mathbf{x}_{T_j}|^{-1}}{\sum_{T_j \ni \mathbf{v}_i} |\mathbf{v}_i - \mathbf{x}_{T_j}|^{-1}}.$$

Reference point position

For any triangle $T = \mathbf{v}_1\mathbf{v}_2\mathbf{v}_3$ and for any diffusion tensor \mathbb{D} the point \mathbf{x}_T is defined as follows:

$$\mathbf{x}_T = \frac{\sum_{i=1}^3 \mathbf{v}_i |\mathbf{n}_{\alpha(i)}| \mathbb{D}}{\sum_{i=1}^3 |\mathbf{n}_{\alpha(i)}| \mathbb{D}} \quad \text{where } |\mathbf{n}_{\alpha(i)}| \mathbb{D} = (\mathbb{D} \mathbf{n}_{\alpha(i)} \cdot \mathbf{n}_{\alpha(i)})^{1/2} \quad (3)$$

and $\mathbf{n}_{\alpha(i)}$ is the outward normal to the edge $e_{\alpha(i)}$ opposite to the vertex \mathbf{v}_i .

Iterative solution

The substitution of flux (2) into equation (1) yields the nonlinear system:

$$\mathbf{A}(C)C = F. \quad (4)$$

We use the simplest Picard iterations: initial vector $C^0 \in \mathbb{R}^{N_T}$, $C^0 \geq 0$,

$$\text{solve } \mathbf{A}(C^{k-1})C^k = F, \quad k = 1, 2, \dots \quad (5)$$

Matrix $\mathbf{A}(C^{k-1})$ has at most **four** non-zeros in each row.

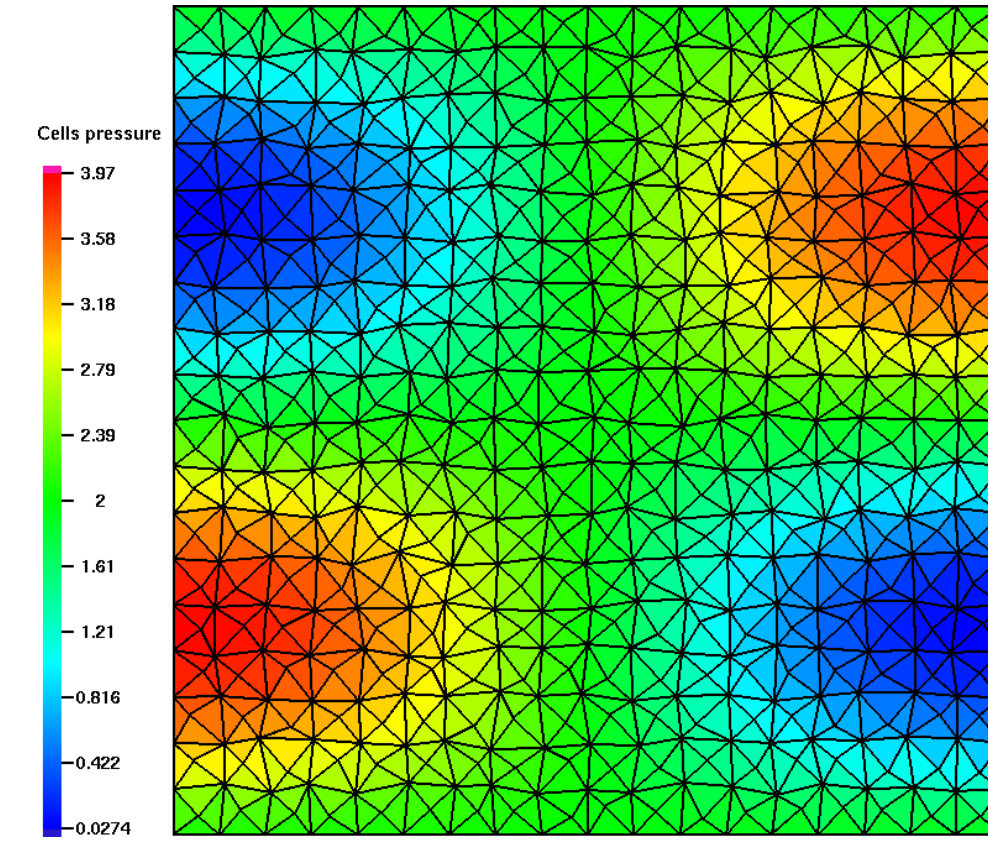
Theoretical result

Let \mathbf{x}_{T_i} be defined by (3) and $F_{T_i} \geq 0$, $C_{T_i}^0 \geq 0$, $i = 1, \dots, N_T$. Then all iterates C^k of method (5) are **non-negative**:

$$C_{T_i}^k \geq 0, \quad i = 1, \dots, N_T, \quad k = 1, 2, \dots$$

The proof is based on the fact that if \mathbf{x}_{T_i} are defined by (3) then A_e^+ and A_e^- in (2) are positive.

Numerical Test I: smooth solution



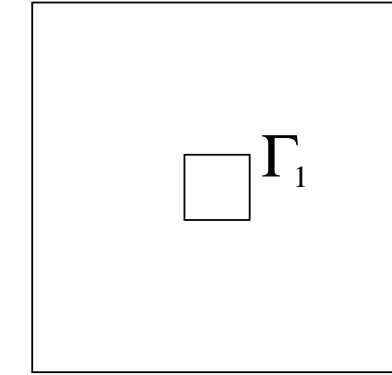
$$C(x, y) = 2\cos(\pi x)\sin(2\pi y) + 2$$

$$-\operatorname{div} \operatorname{grad} C + C = f \quad \text{in } \Omega = [0; 1]^2$$

h	$\ C - C_h\ _2$	$\ \mathbf{q} - \mathbf{q}_h\ _2$
1/18	$9.43e-3$	$3.25e-2$
1/36	$2.33e-3$	$8.48e-3$
1/72	$6.00e-4$	$2.73e-3$
1/144	$1.57e-4$	$9.17e-4$

- Second order convergence in discrete L_2 norms for both C and \mathbf{q} when the solution is smooth.

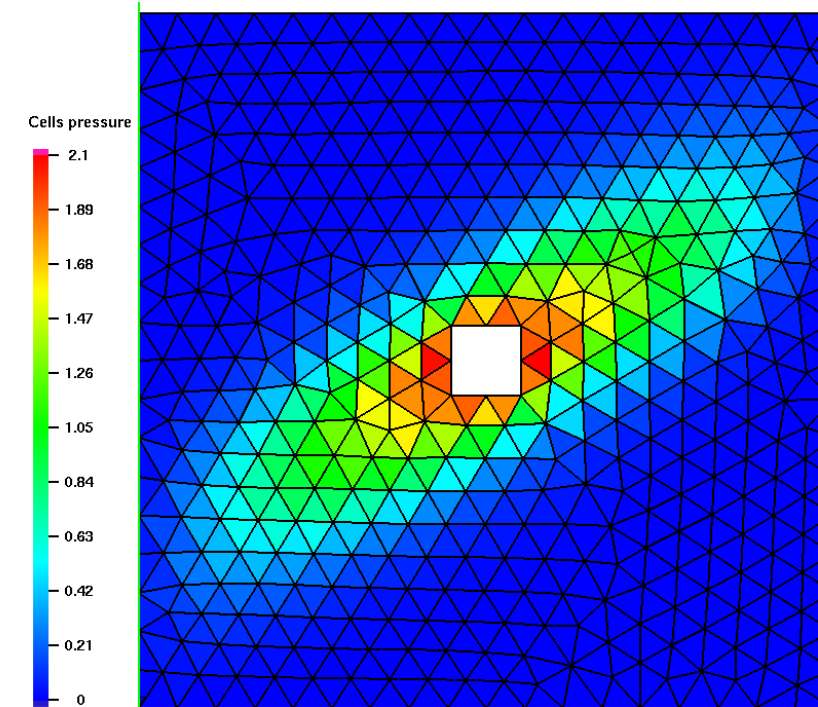
Numerical Test II: anisotropic solution



$$-\operatorname{div} \mathbb{D} \operatorname{grad} C = 0 \quad \text{in } \Omega, \quad C = 0 \text{ on } \Gamma_0, \quad C = 2 \text{ on } \Gamma_1.$$

$$\mathbb{D} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} k_1 & 0 \\ 0 & k_2 \end{pmatrix} \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

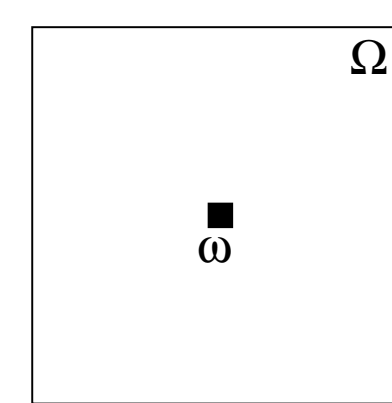
$$k_1 = 100 \quad k_2 = 1 \quad \theta = \pi/6$$



h	$\ C - C_h\ _\infty$	$\ C - C_h\ _2$
1/18	$1.11e-0$	$9.70e-2$
1/36	$8.66e-1$	$5.11e-2$
1/72	$6.04e-1$	$2.53e-2$
1/144	$3.38e-1$	$1.22e-2$

- First order convergence in the discrete L_2 norm for C variable when the solution is nonsmooth and highly anisotropic.

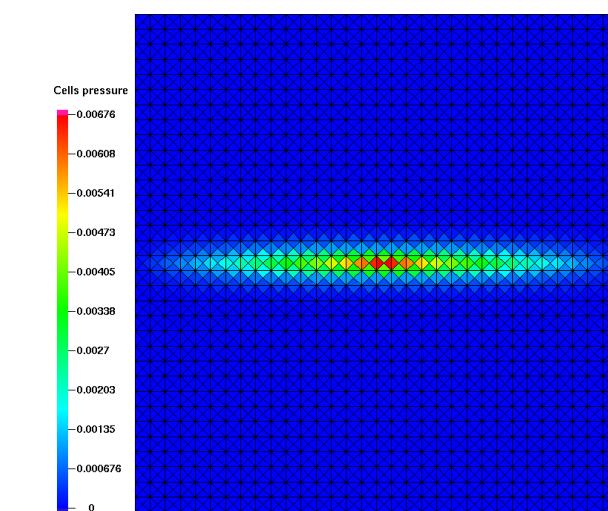
Numerical Test III: positivity



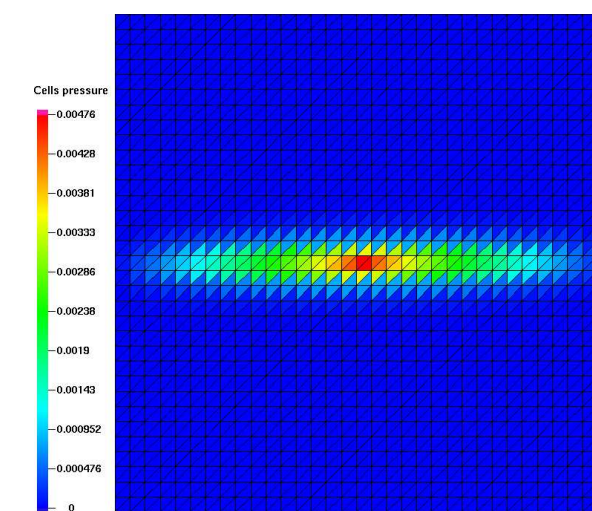
$$-\operatorname{div} \mathbb{D} \operatorname{grad} C = f \quad \text{in } \Omega, \quad C = 0 \text{ on } \partial\Omega \quad \Omega = [0, 1]^2$$

$$f = \begin{cases} \frac{1}{|\omega|} & \text{in } \omega \\ 0 & \text{otherwise} \end{cases} \quad \omega = [0.5 - h/2, 0.5 + h/2]^2$$

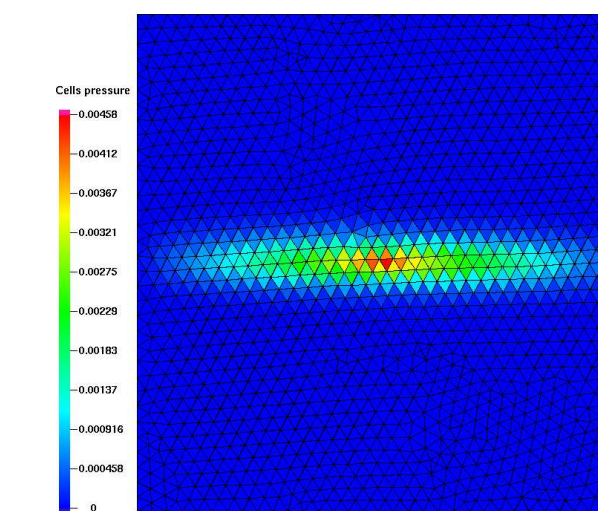
$$k_1 = 1000 \quad k_2 = 1 \quad \theta = 0$$



$$C_{\min} = 0.$$

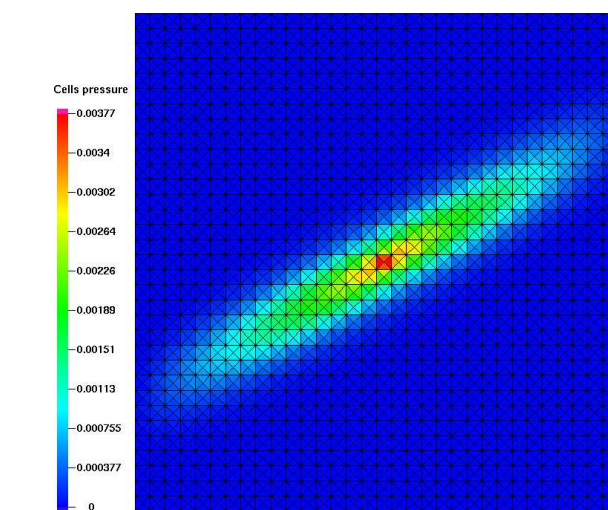


$$C_{\min} = 0.$$

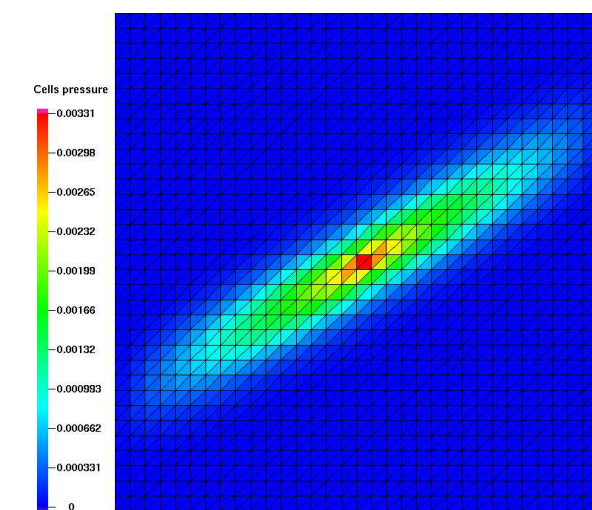


$$C_{\min} = 0.$$

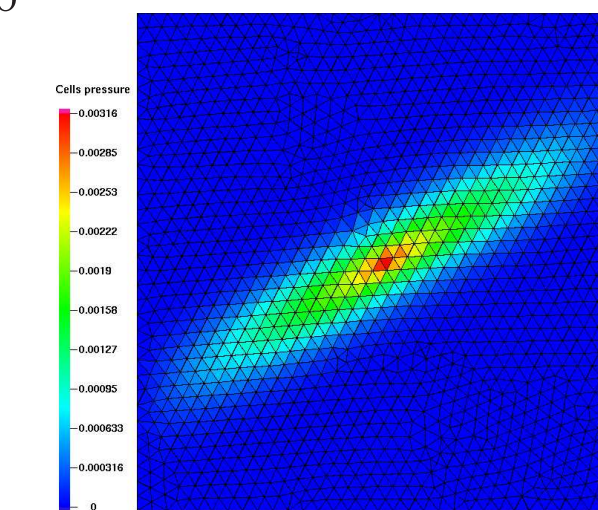
$$k_1 = 1000 \quad k_2 = 1 \quad \theta = \pi/6$$



$$C_{\min} = 0.$$



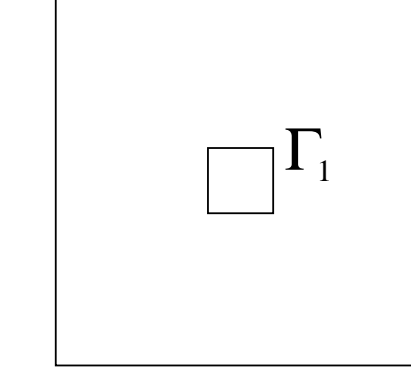
$$C_{\min} = 0.$$



$$C_{\min} = 0.$$

- The solution remains **non-negative** on different types of meshes and for different directions of anisotropy.
- Both RT_0 and P_1 methods produce **negative** C_{\min} in all cases.

Overshooting

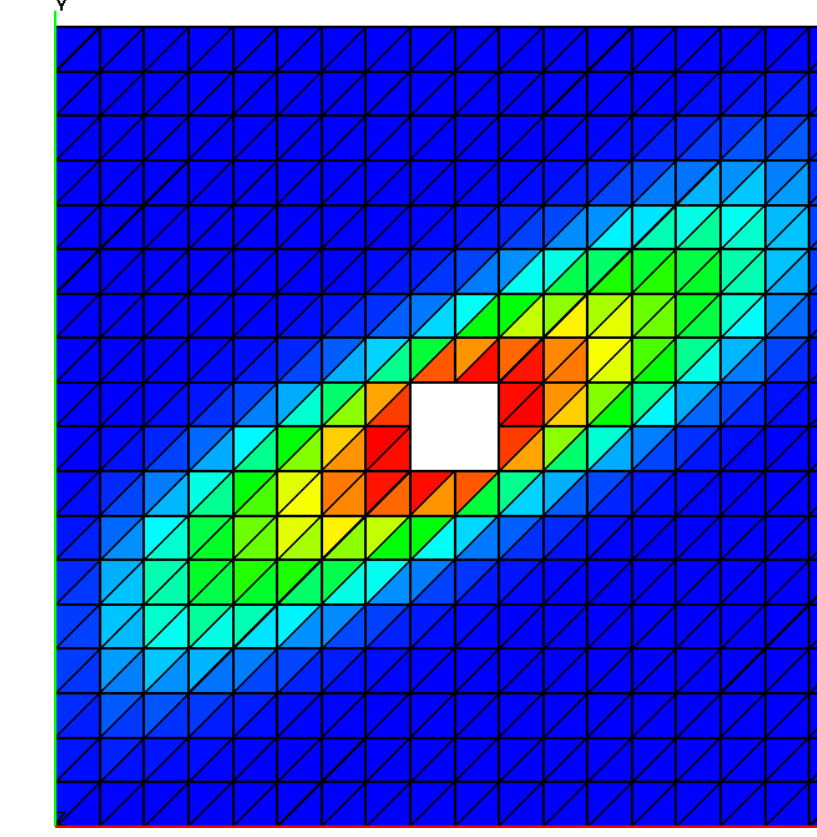


$$-\operatorname{div} \mathbb{D} \operatorname{grad} C = 0 \quad \text{in } \Omega \quad \Omega = [0, 1]^2$$

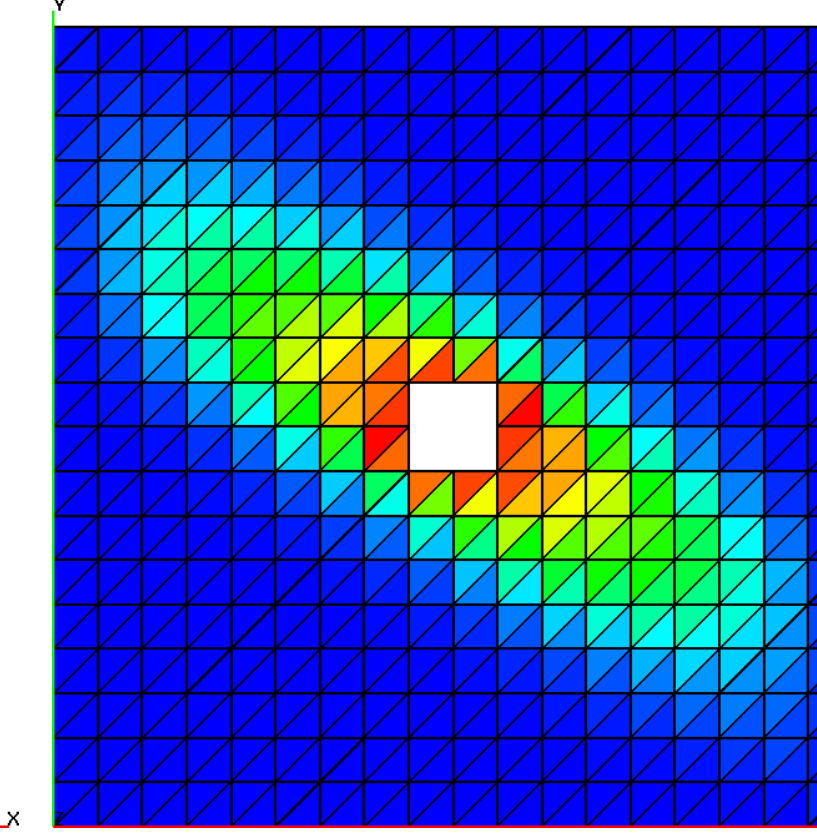
$$C = 0 \quad \text{on } \Gamma_0$$

$$C = 2 \quad \text{on } \Gamma_1$$

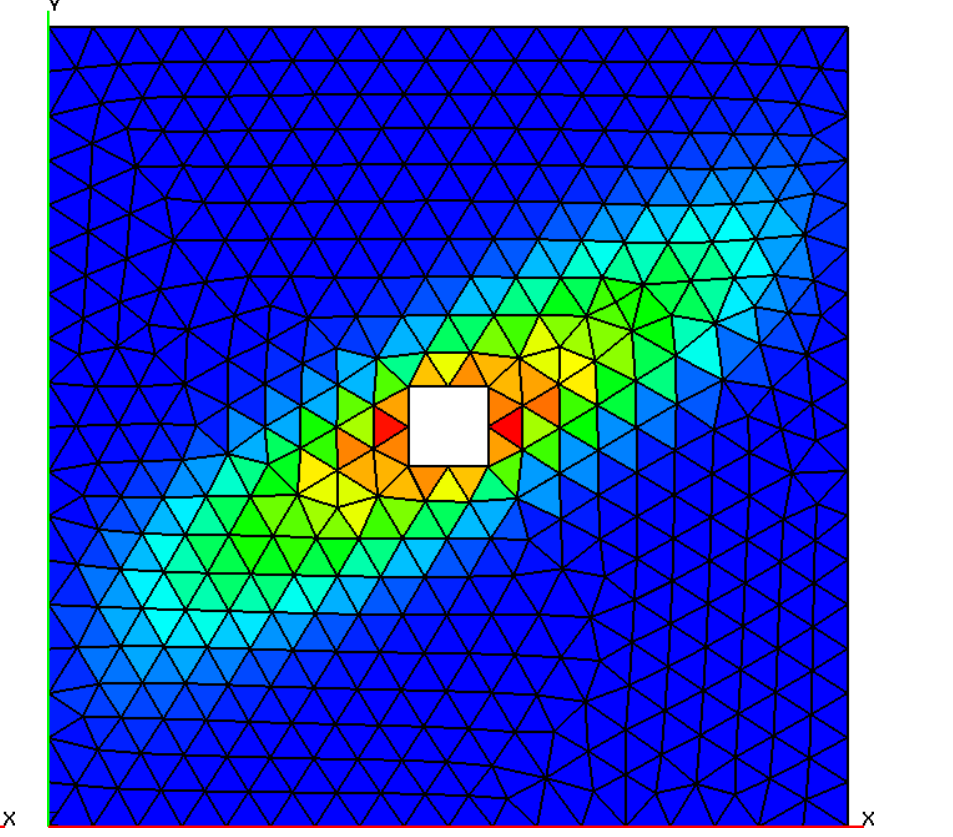
- In the case of highly anisotropic solution overshoots may occur.
- The overshoot values are sensitive to the choice of an interpolation technique.
- Overshooting depends on a mutual orientation of an anisotropic solution and mesh edges.



C_{max}	Interpolation	
$k1/k2$	I_1	I_2
10	1.96	1.96
1000	1.98	1.98



C_{max}	Interpolation	
$k1/k2$	I_1	I_2
10	1.97	1.97
1000	2.95	2.05



C_{max}	Interpolation	
$k1/k2$	I_1	I_2
10	1.99	1.99
1000	2.75	2.14

I_1 – linear interpolation

I_2 – inverse distance weighting interpolation

- Inverse distance weighting interpolation is more stable in the case of highly anisotropic solutions.
- L_2 norm of the overshoot error ($\max\{C_h - 2, 0\}$) behaves like $O(h)$.

Extension to quadrilateral meshes

- Q is a comformal quadrilateral mesh with shape regular cells

$$\operatorname{diam}(Q)/\rho(Q) \leq \text{const} \quad \forall Q \in \mathcal{Q}.$$

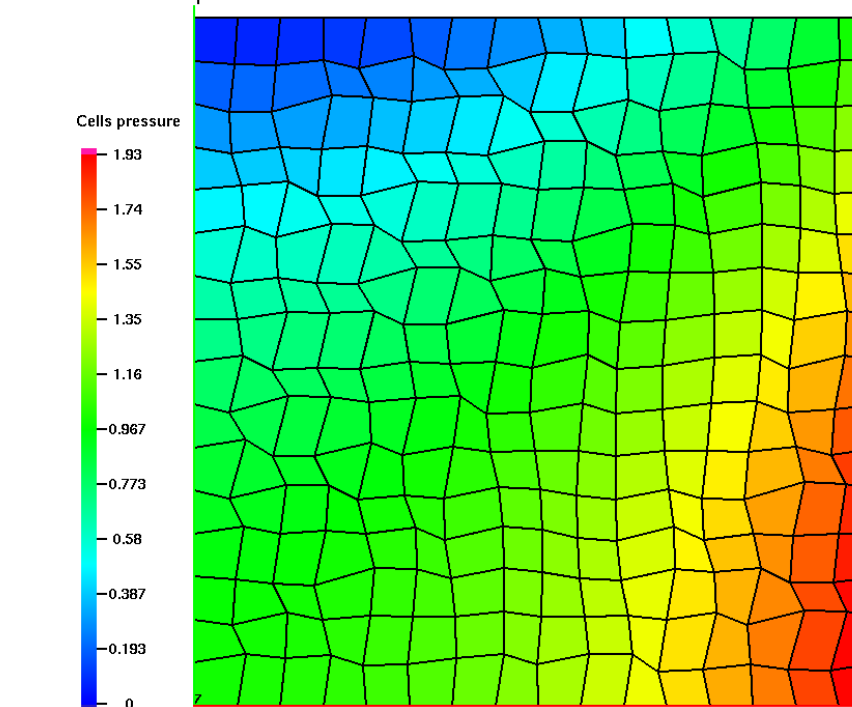
- $\mathbf{x}_Q \in Q$ is a point separated from ∂Q for which Q is star-shaped. For convex or slightly non-convex cells \mathbf{x}_Q may be the mass center.

- \mathbb{D} is isotropic and heterogeneous on \mathcal{Q}

- Each edge may be artificially extended so that coefficients A_e^+ and A_e^- in (2) are positive. Hence the scheme is **monotone**.

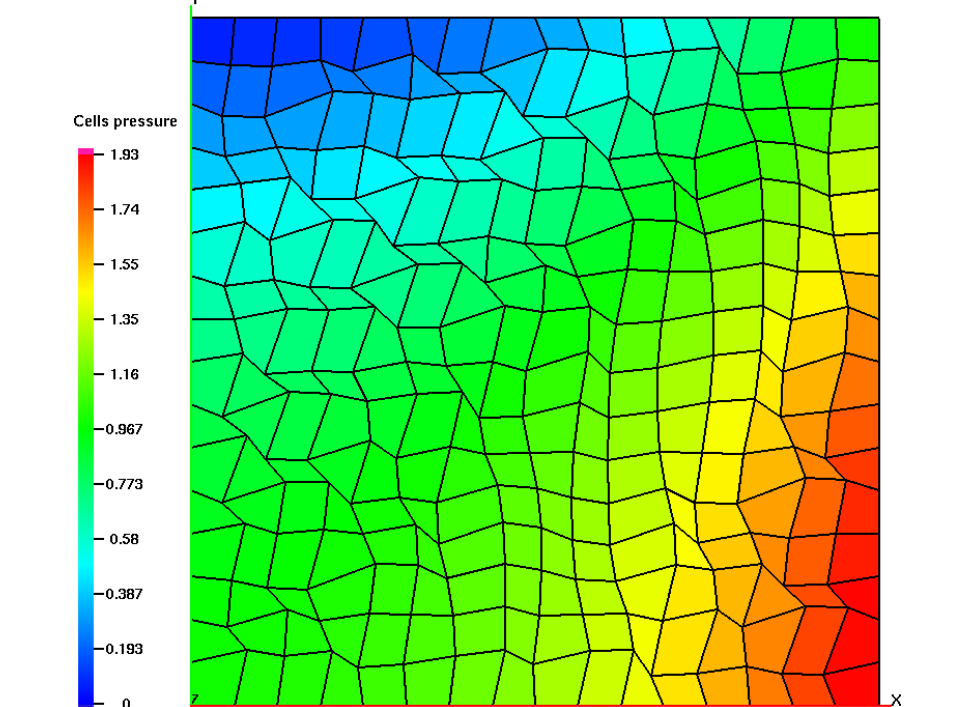
$$C(x, y) = x^2 - y^2 + 1$$

$$-\operatorname{div} \operatorname{grad} C + C = f \quad \text{in } \Omega = [0; 1]^2$$



less distorted mesh

h	$\ C - C_h\ _2$	$\ \mathbf{q} - \mathbf{q}_h\ _2$
1/16	$9.87e-4$	$2.70e-3$
1/32	$2.55e-4$	$7.23e-4$
1/64	$6.38e-5$	$2.27e-4$
1/128	$1.59e-5$	$7.59e-5$



more distorted mesh

h	$\ C - C_h\ _2$	$\ \mathbf{q} - \mathbf{q}_h\ _2$
1/16	$4.14e-3$	$3.18e-2$
1/32	$2.44e-3$	$2.17e-2$
1/64	$1.33e-3$	$1.88e-2$
1/128	$6.99e-4$	$1.16e-2$

- The convergence rate is affected by the distortion degree.
- Matrix $\mathbf{A}(C^{k-1})$ from (5) has at most **five** nonzeros in each row.