

A New Cell-Vertex Reconstruction Method for Finite Volume Schemes

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SHARING HIGHER-ORDER ADVANCED RESEARCH KNOW-HOW on FINITE VOLUME

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Outline

- 1 Motivations
- 2 Cell-Vertex Reconstruction
- 3 Polynomial Reconstructions
- 4 Steady-state Convection-Diffusion-Reaction Problems
- 5 Anisotropic Diffusion Problems
- 6 Conclusions

Motivations

➤ Why a second-order scheme?

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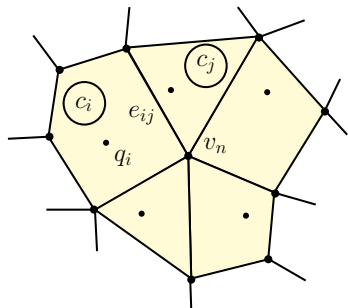
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- 😊 Simple reconstruction of the gradient
- 😊 Simple integration formulas on cells

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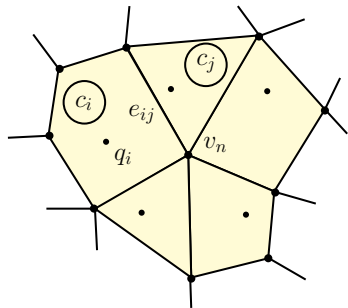
Notations

- c_i and $|c_i|$, $i = 1, \dots, I$ – cell and its area



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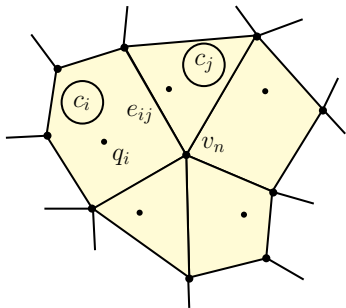
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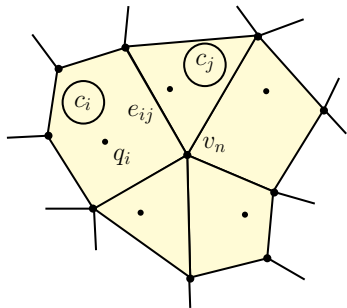
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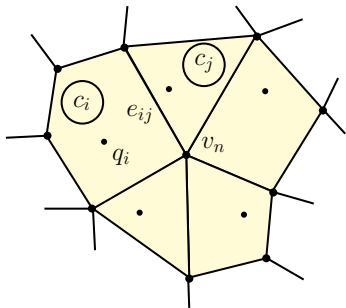
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- Stencil:

$$\mu(n) = \{\text{indices of the cells which share } v_n\}$$

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👉 Goal:

Cell (Φ) \rightarrow Vertex (Ψ)

Cell-Vertex Reconstruction

The Method

- Frink's method (1991): linear combination (☹ First-order approximation!)

$$\psi_n = \sum_{i \in \mu(n)} \beta_{ni} \phi_i$$

$$\text{with } \beta_{ni} = \frac{\overline{q_i v_n}}{\sum_{i \in \mu(n)} \overline{q_i v_n}}$$

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Coefficients = Minimization Functional + Affine Constraints

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- Chandrashekar et al.'s method (2013): extended Rauch et al.'s method

Coefficients = Minimization Functional + Affine Constraints + Weights

Cell-Vertex Reconstruction

The Method

- Coudière et al.'s method (1999): affine reconstruction

$$\psi_n = av_{nx} + bv_{ny} + c$$

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Costa, Clain and Machado's method

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- Linear combination:

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$$\psi_n = \sum_{i \in \mu(n)} \beta_{ni} \phi_i$$

$$B^n = (\beta_{ni})_{i \in \mu(n)}$$

- Affine constraints:

$$\Lambda_1(B^n) = \sum_{i \in \mu(n)} \beta_{ni}, \quad \Lambda_2(B^n) = \sum_{i \in \mu(n)} \beta_{ni} x_{ni}, \quad \Lambda_3(B^n) = \sum_{i \in \mu(n)} \beta_{ni} y_{ni}$$

$$\Lambda_1(B^n) = 1$$

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where $x_{ni} = q_{ix} - v_{nx}$, $y_{ni} = q_{iy} - v_{ny}$

Cell-Vertex Reconstruction

Costa, Clain and Machado's method

- Quadratic functional:

$$E(B^n) = \frac{1}{2} \sum_{i \in \mu(n)} \omega_{ni} (\beta_{ni} - \theta_{ni})^2$$

$$\sum_{i \in \mu(n)} \theta_{ni} = 1$$

ω_{ni} – positive weights, θ_{ni} – targets

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- Lagrange multipliers: find vector $\Lambda^n = (\lambda_{n1}, \lambda_{n2}, \lambda_{n3})$ such that

$$\beta_{ni} = \theta_{ni} - \frac{1}{\omega_{ni}} (\lambda_{n1} + \lambda_{n2} x_{ni} + \lambda_{n3} y_{ni}), \quad i \in \mu(n)$$

- System of linear equations $\rightarrow \Lambda^n \rightarrow B^n$

Cell-Vertex Reconstruction

Positivity principle preserving

- **Positivity principle:** positive cell values ϕ_i , $i \in \mu(n)$, yield a positive vertex value ψ_n

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- To guarantee the positivity principle we seek positive coefficients, because

$$\text{if } \beta_{ni} \geq 0, \phi_i \geq 0 \therefore \psi_n = \sum_{i \in \mu(n)} \beta_{ni} \phi_i \geq 0$$

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- 1 Positive target values

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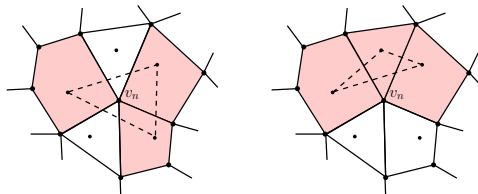
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- 2 Choose a new stencil consisting of three cells of $\mu(n)$



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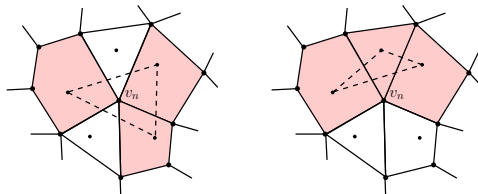
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- 3 Best configuration? $B^n = (1/3, 1/3, 1/3)$

Cell-Vertex Reconstruction

3D extension

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- Affine constraints:

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$$\Lambda_4(B^n) = \sum_{i \in \mu(n)} \beta_{ni} z_{ni}$$

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- Quadratic functional + Lagrange Multipliers

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- Treatment of the boundary vertices:
 - Dirichlet vertex: $\psi_n = \phi_D(v_n)$
 - Neumann vertex (2 different techniques):
 - interpolation technique as explained before
 - interpolation technique with ghost cells + Neumann conditions

Polynomial Reconstructions

Polynomial reconstructions on cells

Let us assume vectors Φ and Ψ are given!

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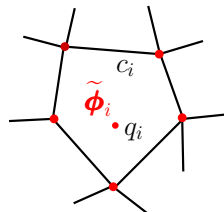
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- First-degree polynomial associated to the cell c_i :

$$\phi_i(x, y) = \phi_i + \mathcal{R}_{i,x}(x - q_{ix}) + \mathcal{R}_{i,y}(y - q_{iy})$$

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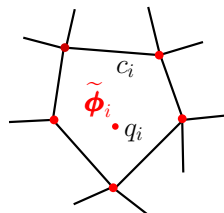
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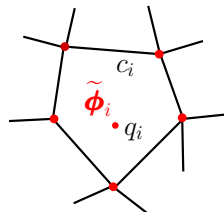
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- $\tilde{\phi}_i(x, y)$ – associated polynomial



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Polynomial reconstructions on edges

- First-degree polynomial associated to the edge e_{ij} :

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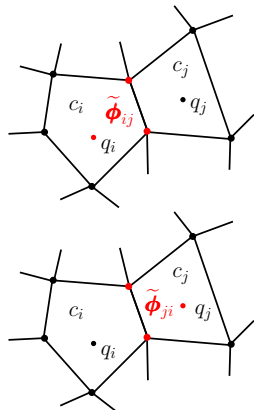
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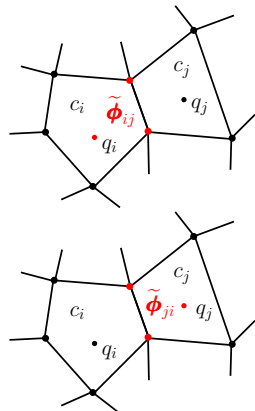
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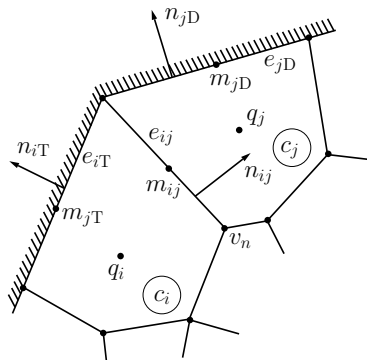
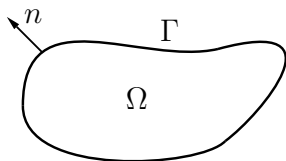
$$S_{ij} = \{\text{indices of the vertices of } e_{ij}\}$$

- Find $\tilde{\mathcal{R}}_{ijx}$ and $\tilde{\mathcal{R}}_{ijy}$, such that $\tilde{\phi}_{ij}(x, y)$ interpolates ϕ_i and $\psi_n, n \in S_{ij}$
- $\tilde{\phi}_{ji}(x, y)$ is also performed
- The same procedure for the boundary edges



Steady-state Convection-Diffusion-Reaction Problems

Mesh



- Domain Ω , boundary $\Gamma = \Gamma_D \cup \Gamma_P \cup \Gamma_T$
- $\nu(i) = \{\text{indices of the cells/boundaries which share an edge with } c_i\}$
- $|e_{ij}|$, $i = 1 \dots, I$, $j \in \nu(i)$ – length of e_{ij}

Steady-state Convection-Diffusion-Reaction Problems

Formulation

$$\nabla \cdot (V\phi - \kappa \nabla \phi) + r\phi = f, \text{ in } \Omega$$

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- $\phi \equiv \phi(x, y)$ – unknown
- $V = (u, v) \equiv (u(x, y), v(x, y))$ – velocity
- $\kappa \equiv \kappa(x, y)$ – diffusion coefficient
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- Dirichlet: $\phi = \phi_D(x, y)$, on Γ_D

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- Dirichlet: $\phi = \phi_D(x, y)$, on Γ_D
- Partial Neumann: $-\kappa \nabla \phi \cdot n = g_P(x, y)$, on Γ_P

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- Dirichlet: $\phi = \phi_D(x, y)$, on Γ_D
- Partial Neumann: $-\kappa \nabla \phi \cdot n = g_P(x, y)$, on Γ_P
- Total Neumann: $V \cdot n\phi - \kappa \nabla \phi \cdot n = g_T(x, y)$, on Γ_T

Steady-state Convection-Diffusion-Reaction Problems

Finite volume discretization

- Integration over cell c_i and applying the divergence theorem

$$\sum_{j \in \nu(i)} \frac{|e_{ij}|}{|c_i|} \frac{1}{|e_{ij}|} \int_{e_{ij}} (V \cdot n_{ij} \phi - \kappa \nabla \phi \cdot n_{ij}) \, ds + \frac{1}{|c_i|} \int_{c_i} r \phi \, dX - \frac{1}{|c_i|} \int_{c_i} f \, dX = 0$$

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- Generic finite volume scheme:

$$\sum_{j \in \nu(i)} \frac{|e_{ij}|}{|c_i|} \mathcal{F}_{ij}(\Phi) + \mathcal{R}_i(\Phi) - f_i = \mathcal{O}(h^2), \quad i = 1, \dots, I$$

- \mathcal{F}_{ij} – convective and diffusive fluxes
- \mathcal{R}_i – mean reactive part
- f_i – mean source term

Steady-state Convection-Diffusion-Reaction Problems

Second-order finite volume scheme – numerical fluxes

- Inner edge e_{ij} :

$$\mathcal{F}_{ij} = [V(m_{ij}) \cdot n_{ij}]^+ \tilde{\phi}_i(m_{ij}) + [V(m_{ij}) \cdot n_{ij}]^- \tilde{\phi}_j(m_{ij}) - \kappa(m_{ij}) \nabla \check{\phi}_{ij}(m_{ij}) \cdot n_{ij}$$

where

$$\check{\phi}_{ij} = \check{\phi}_{ji} = \sigma_{ij} \tilde{\phi}_{ij} + \sigma_{ji} \tilde{\phi}_{ji}, \quad \sigma_{ij} = \frac{|c_i|}{|c_i| + |c_j|}, \quad \sigma_{ji} = \frac{|c_j|}{|c_i| + |c_j|}$$

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Second-order finite volume scheme – numerical fluxes

- Inner edge e_{ij} :

$$\mathcal{F}_{ij} = [V(m_{ij}) \cdot n_{ij}]^+ \tilde{\phi}_i(m_{ij}) + [V(m_{ij}) \cdot n_{ij}]^- \tilde{\phi}_j(m_{ij}) - \kappa(m_{ij}) \nabla \check{\phi}_{ij}(m_{ij}) \cdot n_{ij}$$

where

$$\check{\phi}_{ij} = \check{\phi}_{ji} = \sigma_{ij} \tilde{\phi}_{ij} + \sigma_{ji} \tilde{\phi}_{ji}, \quad \sigma_{ij} = \frac{|c_i|}{|c_i| + |c_j|}, \quad \sigma_{ji} = \frac{|c_j|}{|c_i| + |c_j|}$$

- Dirichlet boundary edge e_{iD} :

$$\mathcal{F}_{iD} = [V(m_{iD}) \cdot n_{iD}]^+ \tilde{\phi}_i(m_{iD}) + [V(m_{iD}) \cdot n_{iD}]^- \phi_D(m_{iD}) - \kappa(m_{iD}) \nabla \check{\phi}_{iD}(m_{iD}) \cdot n_{iD}$$

Steady-state Convection-Diffusion-Reaction Problems

Second-order finite volume scheme – numerical fluxes

- Inner edge e_{ij} :

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- Partial Neumann boundary edge e_{iP} : $\mathcal{F}_{iP} = V(m_{iP}) \cdot n_{iP} \tilde{\phi}_i(m_{iP}) + g_P(m_{iP})$

Steady-state Convection-Diffusion-Reaction Problems

Second-order finite volume scheme – numerical fluxes

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$$\mathcal{F}_{ij} = [V(m_{ij}) \cdot n_{ij}]^+ \tilde{\phi}_i(m_{ij}) + [V(m_{ij}) \cdot n_{ij}]^- \tilde{\phi}_j(m_{ij}) - \kappa(m_{ij}) \nabla \check{\phi}_{ij}(m_{ij}) \cdot n_{ij}$$

where

$$\check{\phi}_{ij} = \check{\phi}_{ji} = \sigma_{ij} \tilde{\phi}_{ij} + \sigma_{ji} \tilde{\phi}_{ji}, \quad \sigma_{ij} = \frac{|c_i|}{|c_i| + |c_j|}, \quad \sigma_{ji} = \frac{|c_j|}{|c_i| + |c_j|}$$

- Dirichlet boundary edge e_{iD} :

$$\mathcal{F}_{iD} = [V(m_{iD}) \cdot n_{iD}]^+ \tilde{\phi}_i(m_{iD}) + [V(m_{iD}) \cdot n_{iD}]^- \phi_D(m_{iD}) - \kappa(m_{iD}) \nabla \tilde{\phi}_{iD}(m_{iD}) \cdot n_{iD}$$

- Partial Neumann boundary edge e_{iP} : $\mathcal{F}_{iP} = V(m_{iP}) \cdot n_{iP} \tilde{\phi}_i(m_{iP}) + g_P(m_{iP})$
- Total Neumann boundary edge e_{iT} : $\mathcal{F}_{iT} = g_T(m_{iT})$

Steady-state Convection-Diffusion-Reaction Problems

Finite volume scheme – reactive part and source term

- \mathcal{R}_i for cell c_i

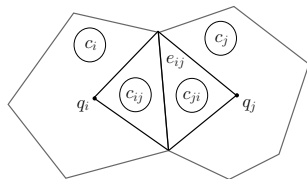
$$\mathcal{R}_i = r(q_i)\phi_i$$

or

$$\mathcal{R}_i = \frac{1}{|c_i|} \left[\sum_{j \in \nu(i)} \frac{|c_{ij}|}{3} \left(\sum_{n \in S_{ij}} r(v_n)\psi_n + r(q_i)\phi_i \right) \right]$$

- f_i for cell c_i

$$f_i = \frac{1}{|c_i|} \left[\sum_{j \in \nu(i)} \frac{|c_{ij}|}{3} \left(\sum_{n \in S_{ij}} f(v_n) + f(q_i) \right) \right]$$



Steady-state Convection-Diffusion-Reaction Problems

Residual scheme

☞ \mathcal{F}_{ij} and \mathcal{R}_i linearly depend on vector Φ

Steady-state Convection-Diffusion-Reaction Problems

Residual scheme

- ☞ \mathcal{F}_{ij} and \mathcal{R}_i linearly depend on vector Φ
- Affine operator $\Phi \rightarrow \mathcal{G}_i(\Phi)$ for each cell $c_i, i = 1, \dots, I$

$$\mathcal{G}_i(\Phi) = \sum_{j \in \nu(i)} \frac{|e_{ij}|}{|c_i|} \mathcal{F}_{ij}(\Phi) + \mathcal{R}_i(\Phi) - f_i$$

Steady-state Convection-Diffusion-Reaction Problems

Residual scheme

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- $\mathcal{G}(\Phi) = (\mathcal{G}_i(\Phi))_{i=1, \dots, I}$ is an affine operator from \mathbb{R}^I into \mathbb{R}^I

Steady-state Convection-Diffusion-Reaction Problems

Residual scheme

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- $\mathcal{G}(\Phi) = (\mathcal{G}_i(\Phi))_{i=1, \dots, I}$ is an affine operator from \mathbb{R}^I into \mathbb{R}^I
- $\mathcal{G}(\Phi) = 0_I$ provides the solution Φ^*

Steady-state Convection-Diffusion-Reaction Problems

Residual scheme

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- GMRES procedure to solve the affine problem (free-matrix method)

Steady-state Convection-Diffusion-Reaction Problems

Residual scheme

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- $\mathcal{G}(\Phi) = (\mathcal{G}_i(\Phi))_{i=1, \dots, I}$ is an affine operator from \mathbb{R}^I into \mathbb{R}^I
- $\mathcal{G}(\Phi) = 0_I$ provides the solution Φ^*
- GMRES procedure to solve the affine problem (free-matrix method)
- Preconditioning matrix based on a Patankar-like discretization

Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – Criteria

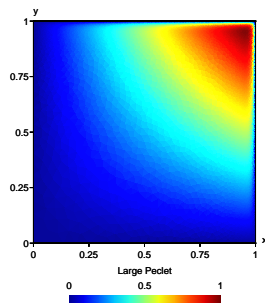
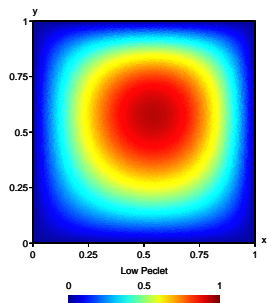
- Exact solution: $\phi_i = \phi(q_i)$, $i = 1, \dots, I$
- Numerical solution $\Phi^* = (\phi_i^*)_{i=1, \dots, I}$
- Relative discrete L^2 -norm error

$$E_2 = \left(\frac{\sum_{i=1}^I |c_i| (\phi_i - \phi_i^*)^2}{\sum_{i=1}^I |c_i| \phi_i^*} \right)^{\frac{1}{2}}$$

Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – Convection-diffusion problem

- $\Omega =]0, 1[^2$
- $\Gamma_D = \Gamma$
- $\phi_D(x, y) = 0$, on Γ_D
- $V = (u, v)$, $\kappa = 1$
- $\phi(x, y) = C\alpha(x)\beta(y)$
- $f(x, y) = C(\alpha(x) + \beta(y))$



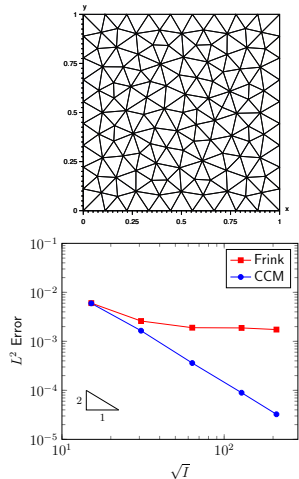
$$\alpha(x) = \frac{1}{u} \left(x - \frac{e^{ux} - 1}{e^u - 1} \right), \quad \beta(y) = \frac{1}{v} \left(y - \frac{e^{vy} - 1}{e^v - 1} \right)$$

- Low Péclet number: $V = (1, 2)$, $C = 65$
- Large Péclet number: $V = (100, 100)$, $C = 11236$

Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – Convection-diffusion problem

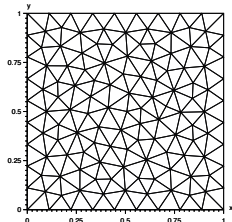
Low Péclet



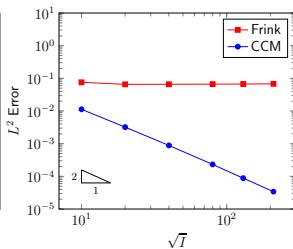
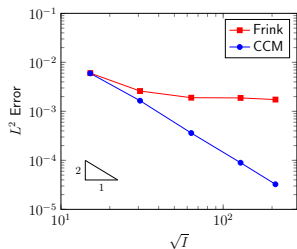
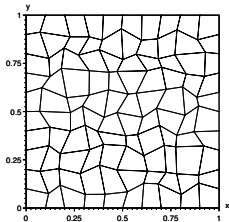
Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – Convection-diffusion problem

Low Péclet



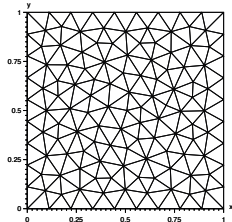
Low Péclet



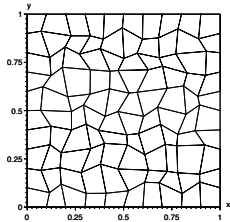
Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – Convection-diffusion problem

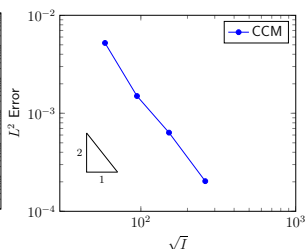
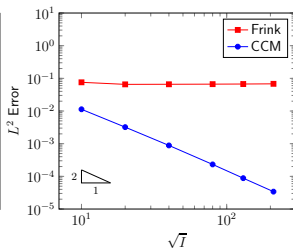
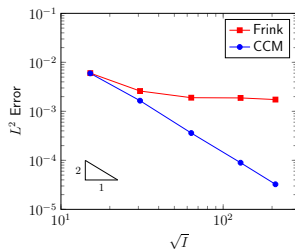
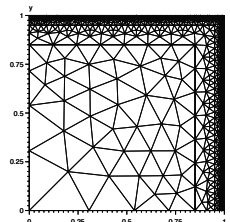
Low Péclet



Low Péclet



Large Péclet



Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – Convection-diffusion problem

- Random value $\xi_{ni} \in [0, 1]$
- Random point on c_i :

$$p_i = \frac{\sum_{n \in S_i} \xi_{ni} v_n}{\sum_{n \in S_i} \xi_{ni}}$$

- Reference cell point of c_i :

$$q_i = m_i + \alpha(p_i - m_i)$$

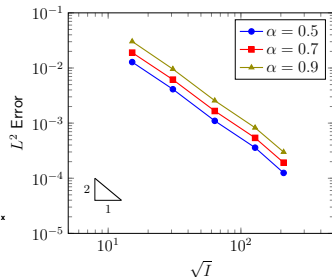
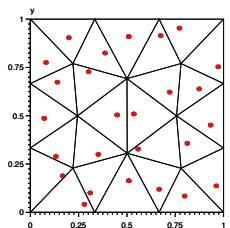
- $\alpha \in [0, 1[$ – deformation factor

Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – Convection-diffusion problem

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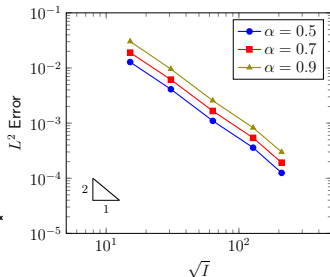
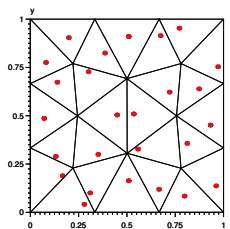
- $\alpha \in [0, 1[$ – deformation factor

Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – Convection-diffusion problem

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- Random point on c_i :

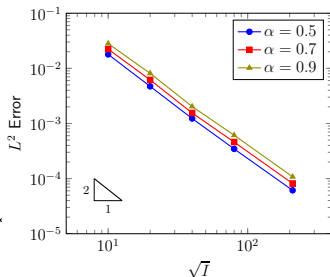
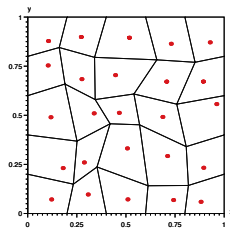
$$p_i = \frac{\sum_{n \in S_i} \xi_{ni} v_n}{\sum_{n \in S_i} \xi_{ni}}$$



- Reference cell point of c_i :

$$q_i = m_i + \alpha(p_i - m_i)$$

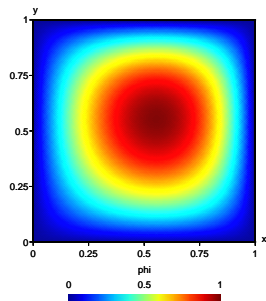
- $\alpha \in [0, 1]$ – deformation factor



Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – Diffusion-reaction problem

- $\Omega =]0, 1[^2$
- $\Gamma_D = \Gamma$
- $\phi_D(x, y) = 0$, on Γ_D
- $\kappa = 1$, $r = 10^6$
- $\phi(x, y) = 3.14x(e^x - e)y(e^y - e)$
- $f = -\kappa\Delta\phi + r\phi$



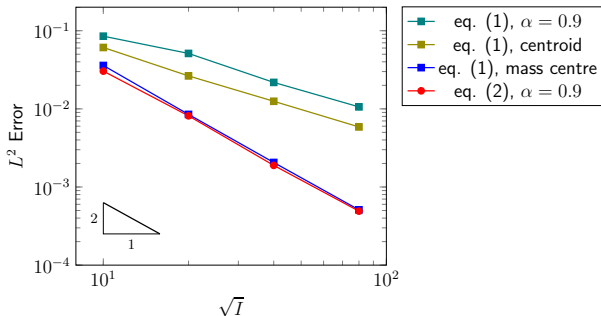
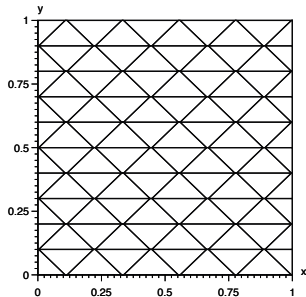
$$\mathcal{R}_i = r(q_i)\phi_i$$

(1) vs

$$\mathcal{R}_i = \frac{1}{|c_i|} \left[\sum_{j \in \nu(i)} \frac{|c_{ij}|}{3} \left(\sum_{n \in \mathcal{S}_{ij}} r(v_n)\psi_n + r(q_i)\phi_i \right) \right] \quad (2)$$

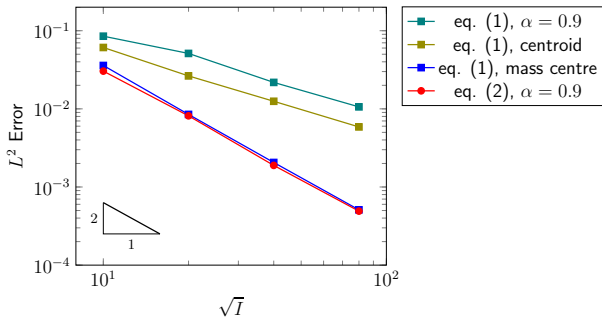
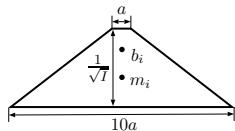
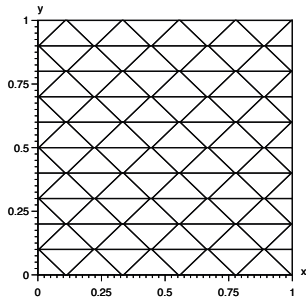
Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – Diffusion-reaction problem



Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – Diffusion-reaction problem



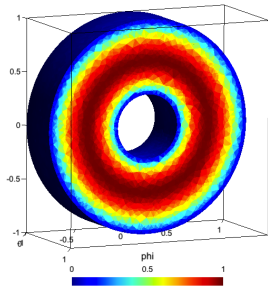
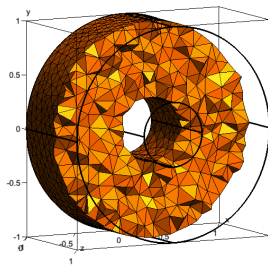
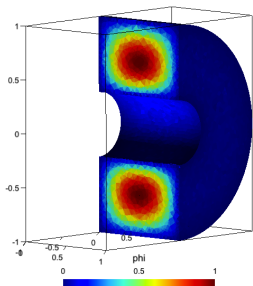
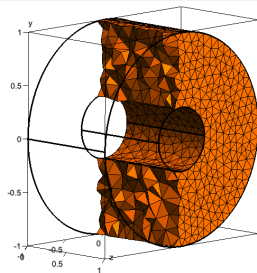
Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – 3D diffusion-reaction problem

- $\Omega = \{(x, y, z) : 0.3 \leq \sqrt{x^2 + y^2} \leq 1, 0 \leq z \leq 1\}$
- $\Gamma_D = \Gamma$
- $\phi_D(x, y, z) = 0$, on Γ_D
- $\kappa = 1, r = 10^6$
- $\phi(x, y, z) = -7.16(z - z^2) \left(\frac{\ln(x^2 + y^2)}{\ln 0.3} + \frac{200}{91}(x^2 + y^2 - 1) \right)$
- $f(x, y, z) = -\kappa \Delta \nabla \phi + r \phi$

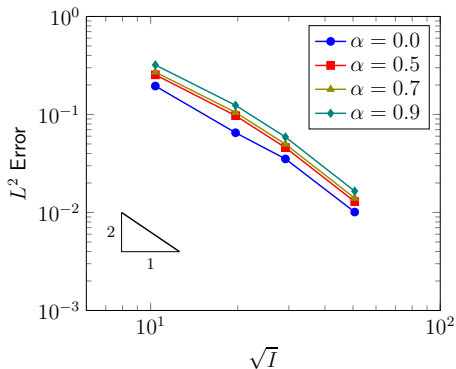
Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – 3D diffusion-reaction problem



Steady-state Convection-Diffusion-Reaction Problems

Numerical Tests – 3D diffusion-reaction problem



Anisotropic Diffusion Problems

Formulation

$$\nabla \cdot (-K \nabla \phi) = f, \text{ in } \Omega$$

- Domain Ω with boundary $\Gamma = \Gamma_D \cup \Gamma_P$
- $\phi \equiv \phi(x, y)$ – unknown
- $K \equiv K(x, y)$ – diffusion tensor, strictly positive definite 2×2 matrix

$$K = \begin{bmatrix} \kappa_{xx} & \kappa_{xy} \\ \kappa_{yx} & \kappa_{yy} \end{bmatrix}$$

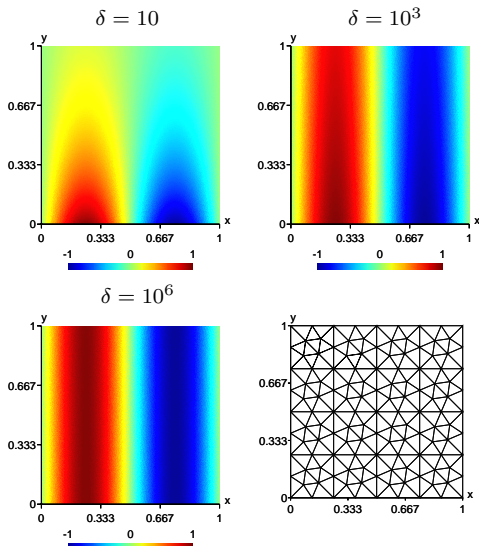
- $f \equiv f(x, y)$ – source term
- Dirichlet: $\phi = \phi_D(x, y)$, on Γ_D
- Partial Neumann: $-K \nabla \phi \cdot n = g_P(x, y)$, on Γ_P

Anisotropic Diffusion Problems

Numerical Tests – Numerical locking problem

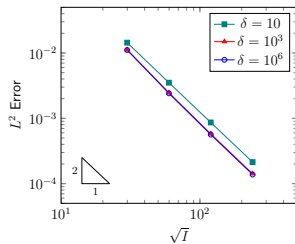
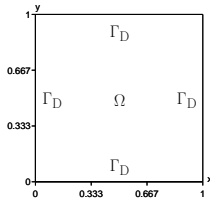
- $\Omega =]0, 1[^2$
- $K = \begin{bmatrix} 1 & 0 \\ 0 & \delta \end{bmatrix}$
- $\delta = 10, 10^3, 10^6$

- $\phi(x, y) = \sin(2\pi x) \exp\left(\frac{-2\pi}{\sqrt{\delta}} y\right)$
- $f(x, y) = 0$



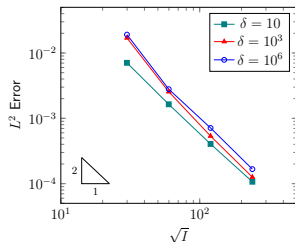
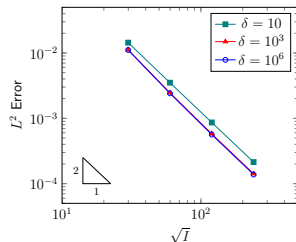
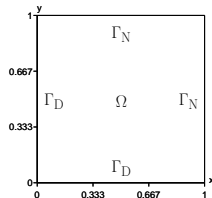
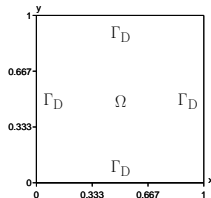
Anisotropic Diffusion Problems

Numerical Tests – Numerical locking problem



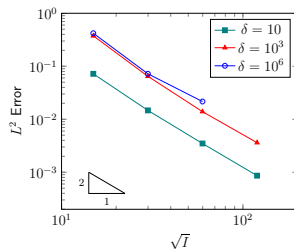
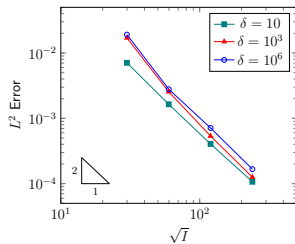
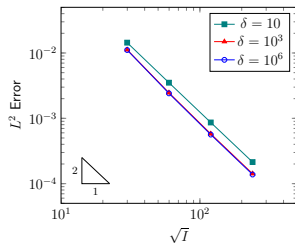
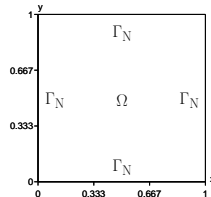
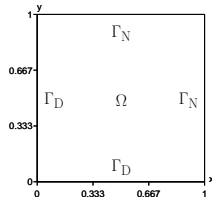
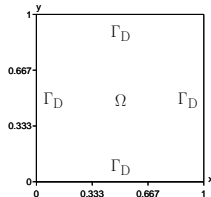
Anisotropic Diffusion Problems

Numerical Tests – Numerical locking problem



Anisotropic Diffusion Problems

Numerical Tests – Numerical locking problem



Conclusions and Perspectives

- ✓ Simple, robust, second-order accuracy

Conclusions and Perspectives

- ✓ Simple, robust, second-order accuracy
- ✓ Unstructured and deformed meshes still preserving the second-order accuracy

Conclusions and Perspectives

- ✓ Simple, robust, second-order accuracy
- ✓ Unstructured and deformed meshes still preserving the second-order accuracy
- ✓ Any reference cell points still preserving the second-order accuracy

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Thank you for your attention!

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