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Coupling of Fluid Flow and Solute Transport Using a Divergence-Free Reconstruction of the Crouzeix-Raviart Element

Problem Description: Transport in a Fluid Flow

The coupling between a fluid flow with velocity $\vec{u}$, pressure p and viscosity η and the steady transport of a dissolved species with concentration c and diffusion coefficient D is governed by the incompressible Navier-Stokes equations

$$-\eta\Delta\vec{u} + (\vec{u}\cdot\nabla)\vec{u} + \nabla p = \vec{f} \text{ in } \Omega, \quad \nabla\cdot\vec{u} = 0 \text{ in } \Omega \quad \text{and} \quad \vec{u} = \vec{u}_D \text{ along } \partial\Omega$$

and the transport equation

$$\nabla\cdot(-D\nabla c + c\vec{u}) = s \text{ in } \Omega \quad \text{and} \quad c = c_D \text{ along } \partial\Omega.$$

The discretisation of the divergence-constraint is a crucial part of the coupling for numerical stability and physical correctness (e.g. maximum principles).

Flow Solver: Modified Crouzeix-Raviart FEM

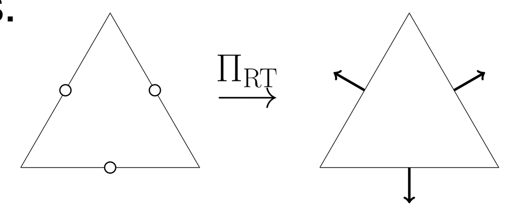
The Navier-Stokes equations are discretised with a modified Crouzeix-Raviart finite element method from [2] on a regular triangulation $\mathcal{T}$. The velocity test functions $\mathrm{CR}(\mathcal{T})$ are piecewise affine, vector-valued functions and continuous in the barycenters of the faces, while the pressure test functions $Q(\mathcal{T})$ are piecewise constant with zero integral mean.

The modified method seeks $(\vec{u}_h, p_h) \in \mathrm{CR}(\mathcal{T}) \times Q(\mathcal{T})$ with $\int_E \vec{u}_D - \vec{u}_h \, ds = 0$ for every boundary face E, and

$$\int_\Omega \eta\nabla\vec{u}_h : \nabla\vec{v}_h \, dx + \int_\Omega (\Pi_{\mathrm{RT}}\vec{u}_h\cdot\nabla)\vec{u}_h\cdot\Pi_{\mathrm{RT}}\vec{v}_h \, dx - \int_\Omega p_h \nabla\cdot\vec{v}_h \, dx = \int_\Omega \vec{f}\cdot\Pi_{\mathrm{RT}}\vec{v}_h \, dx,$$

$$-\int_\Omega q_h \nabla\cdot\vec{u}_h \, dx = 0 \quad \text{for all } (\vec{v}_h, q_h) \in \mathrm{CR}_0(\mathcal{T}) \times Q(\mathcal{T}).$$

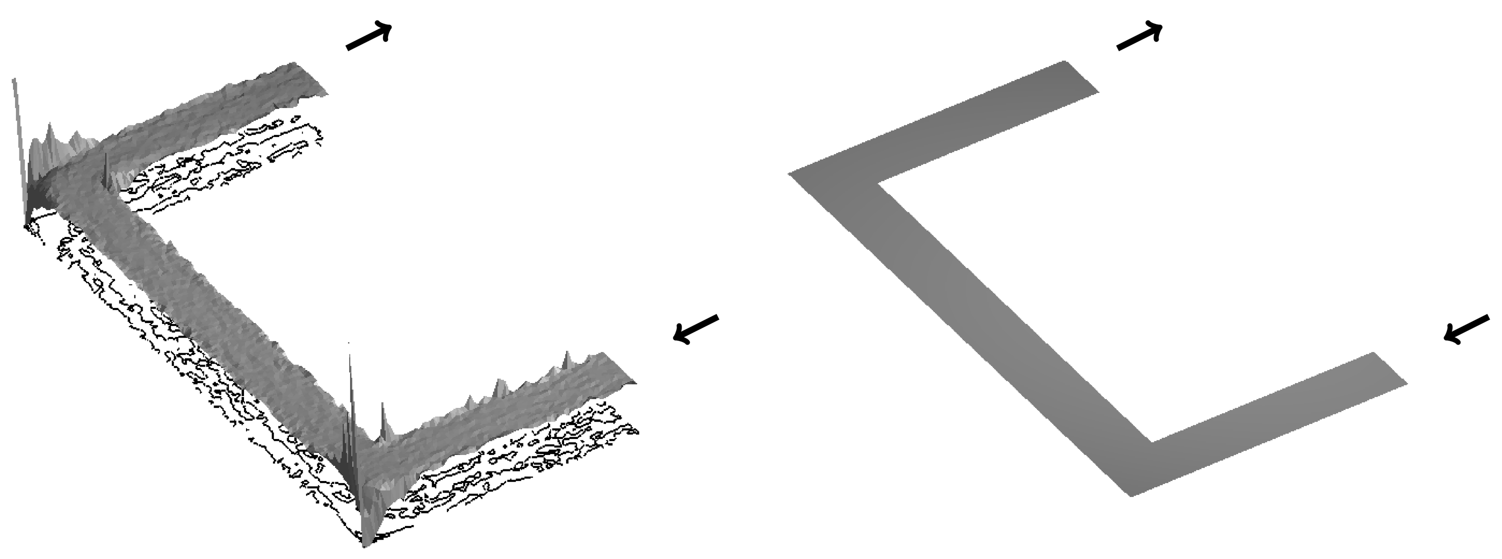
The Fortin interpolation Π_{RT} maps discretely divergence-free test functions to globally divergence-free Raviart-Thomas test functions.



Advantages

- Divergence-free reconstruction ensures preservation of maximum principles for the solute transport (see below).
- Significantly smaller number of degrees of freedom compared to previously introduced divergence-free coupling schemes (e.g. Scott-Vogelius FEM [1]).
- Optimal pressure-independent a priori velocity error estimate. BDM interpolation instead of Π_{RT} yields optimal L^2 error convergence rates [3].

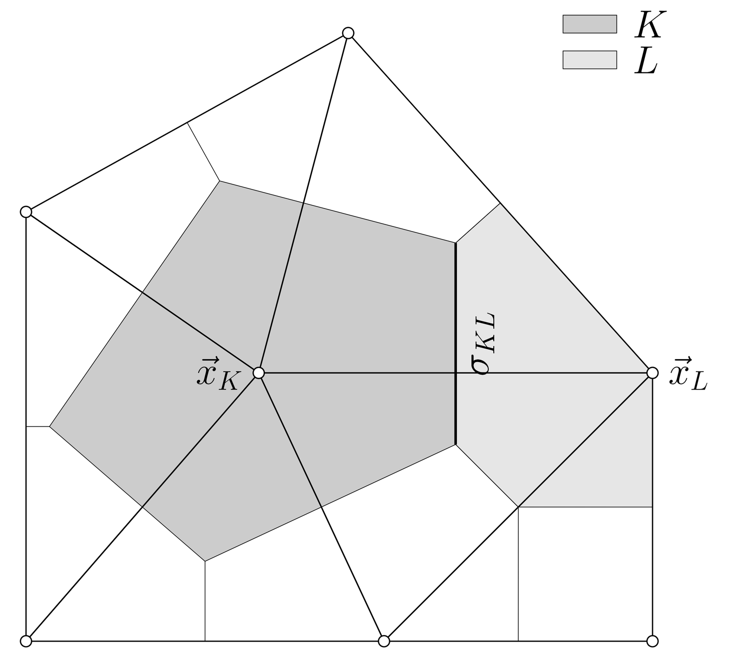
Preservation of Maximum Principle: CR-FEM vs. Modified CR-FEM



Isolines (on the base) and elevation graph of stationary concentration in the longitudinal section of an U-shaped pipe: standard CR-FEM velocity without reconstruction (left) and with modified CR-FEM velocity (right).

Coupling To Solute Transport by FVM

The transport equation is discretised with a finite volume method. Let $\mathcal{P}$ denote a set of points of a Delaunay mesh and let $\mathcal{K}$ denote the associated set of Voronoi cells with facets $\mathcal{F}$.



On every $\sigma_{KL} := \partial K \cap \partial L \in \mathcal{F}$ define

$$u_{\sigma_{KL}} := \int_{\sigma_{KL}} \Pi_{\mathrm{RT}}\vec{u}_h\cdot(\vec{x}_L - \vec{x}_K)\, ds / \left|\sigma_{KL}\right|,$$

$$\tau_{\sigma_{KL}} := \left|\sigma_{KL}\right| / \left|\vec{x}_L - \vec{x}_K\right|.$$

Since $\nabla\cdot\Pi_{\mathrm{RT}}\vec{u}_h = 0$, the fluxes $u_{\sigma_{KL}}$ are discretely divergence-free in the FV sense

$$\sum_{L \text{ neighbour of } K} \tau_{\sigma_{KL}} u_{\sigma_{KL}} = \int_{\partial K} \Pi_{\mathrm{RT}}\vec{u}_h\cdot\vec{n}_K \, dx = \int_K \nabla\cdot\Pi_{\mathrm{RT}}\vec{u}_h \, dx = 0 \quad \text{for all } K \in \mathcal{K}.$$

This guarantees the preservation of maximum principles.

The finite volume scheme seeks $c_h \in P_0(\mathcal{K})$ with $c_K := c_h|_K = c_D(\vec{x}_K)$ for all cells $K \in \mathcal{K}_D$ at the Dirichlet boundary and

$$\sum_{L \text{ neighbour of } K} \tau_{\sigma_{KL}}\, g(c_K, c_L, u_{\sigma_{KL}}) = |K|\, s_K \quad \text{for all } K \in \mathcal{K}_0 := \mathcal{K}\setminus\mathcal{K}_D$$

where $g(c_K, c_L, u_{\sigma_{KL}}) := D\Big(B(u_{\sigma_{KL}}/D)c_K - B(-u_{\sigma_{KL}}/D)c_L\Big)$ define the exponentially fitted flux approximations with Bernoulli function $B(z) = z/(1-e^{-z})$.

Application: Flowcell Simulation

Divergence-free coupling methods allow e.g. to simulate the transport of ions in an electrolyte through a flowcell to validate measurements and determine problem parameters in regimes not covered by the literature. The figure on the left depicts isosurfaces of the ion concentration from [1]. The ultimate goal is to find an efficient discretisation scheme with reasonable complexity.

References

[1] J. Fuhrmann, H. Langmach, and A. Linke. A numerical method for mass conservative coupling between fluid flow and solute transport. *Appl. Numer. Math.*, 61(4):530–553, 2011.

[2] A. Linke. On the role of the Helmholtz decomposition in mixed methods for incompressible flows and a new variational crime. *Comput. Methods Appl. Mech. Engrg.*, 268:782–800, 2014.

[3] C. Brennecke, A. Linke, C. Merdon, and J. Schöberl. Optimal and pressure-independent L2 velocity error estimates for a modified Crouzeix-Raviart Stokes element with BDM reconstructions, 2014. WIAS Preprint 1929.

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