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# The Discretization of Coupled Flows and the Problem of Mass Conservation

## Maximum Principle and Mass Conservation

We are interested in the solution of viscous conservation laws

$$c_t - \nabla \cdot (D \nabla c - c\mathbf{u}) = 0$$

in bounded, polyhedral domains $\Omega \subset \mathbb{R}^d$ with $d = 1, 2, 3$.
We further know that there is a weak maximum principle for the following equation

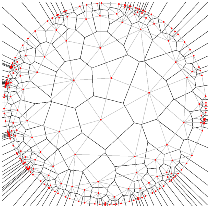
$$u_t + Au = 0 \qquad \text{in } \Omega \text{ for } t > 0$$

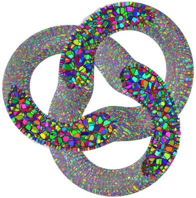
with $u = g$ on $\partial\Omega$, $t \geq 0$, $u(0) = v$ in $\Omega$.
Here

$$Au = -\sum_{k,l=1}^{d} \frac{\partial}{\partial x_k}\left(a_{kl}\frac{\partial u}{\partial x_l}\right) + \sum_{k=1}^{d} b_k \frac{\partial u}{\partial x_k},$$

where the coefficients $a_{kl}, b_k \in C^d(\bar{\Omega})$ are uniformly continuous and $a_{kl}(\mathbf{x})$ is a symmetric and uniformly positive definite matrix on $\bar{\Omega}$.
**Maximum principle**: For $Q_T = \Omega \times (0, T)$, $T > 0$ the maximum and the minimum of a solution $u \in C^2(Q_T) \cap C(\bar{Q}_T)$ over $\bar{Q}_T$ occurs on the parabolic boundary $(\partial\Omega \times [0, T]) \cup \Omega \times \{t = 0\}$.
**Necessary condition that the above conservation law is of this form: $\nabla \cdot \mathbf{u} = 0$!**

## The Voronoi FVM





Discretization of a viscous conservation law for $c$: **vertex-based finite volumes** with

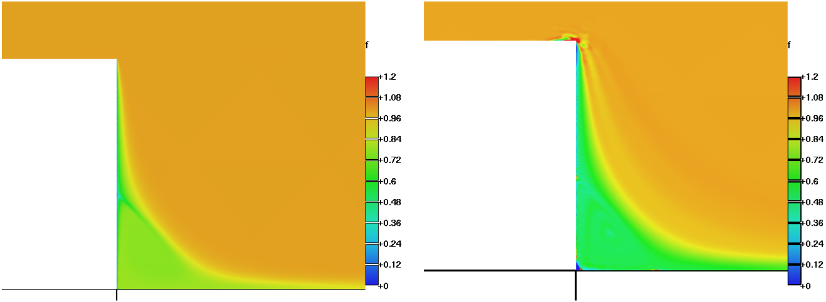
- ▷ Voronoi-boxes as control volumes,
- ▷ $\Rightarrow$ we need boundary conforming Delaunay triangulations in 3D

**FVM approximates**:

$$
\begin{aligned}
\int_K c_t\,dx &= \int_K \nabla\cdot(D\nabla c - c\mathbf{u})\,dx \\
&= \sum_{L\in\mathrm{Neighbour}(K)} \int_{F_{KL}} (D\nabla c - c\mathbf{u})\cdot\mathbf{n}\,ds \\
&\approx -\sum_{L\in\mathrm{Neighbour}(K)} |F_{KL}|\,g(c_K, c_L, U_{KL}, d_{KL}).
\end{aligned}
$$

## An Example

**Weak mass conservation** can lead to considerable errors.




Here, **a steady convection-diffusion** with $D = 1.0 \times 10^{-12}$ is coupled with a backward-facing **Stokes** problem. On the left, we have a **divergence-free FE** method coupled with a FVM. On the right, we have **Taylor-Hood** coupled with the same FVM.

## The Discrete Maximum Principle and the Voronoi FVM

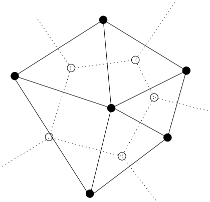
For the vertex-based finite volume discretization, a maximum principle can be proven, if the discretized operator $A$ is a **M-Matrix**:

- positive diagonal entries
- non-positive off-diagonal entries
- non-negative row sums
- at least one positive row sum

**Example: Positivity in the elliptic case**: M-Matrices are **inverse-positive**, i.e., $A^{-1} \geq 0! \Rightarrow$

$$
\begin{aligned}
Ax &= b & \Leftrightarrow \\
x &= A^{-1}b & \Rightarrow \\
b \geq 0 \quad \Rightarrow \quad & x \geq 0.
\end{aligned}
$$

## Example: Convective-Diffusive Flux Splitting (I)

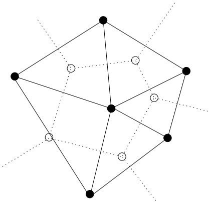


$$-\int_K \nabla\cdot(D\nabla c - c\mathbf{u})\,dx \approx \sum_{L\in\mathrm{Neighbour}(K)} |F_{KL}|\, g(c_K, c_L, U_{KL}, d_{KL})$$

$$= \sum_{L\in\mathrm{Neighbour}(K)} |F_{KL}| \left( D\frac{c_K - c_L}{d_{KL}} + c_K U^+_{KL} - c_L U^-_{KL}\right),$$

with $a^+ := \max(a, 0)$ and $a^- = -\min(a, 0)$.
This **simple upwinding** yields a **first-order scheme** with respect to the consistency of the flux approximation.
For each control volume $K$, we get **one row** of the stiffness-matrix. Obviously, we have **positive diagonal entries**, and **non-positive off-diagonal** entries.

## Example: Convective-Diffusive Flux Splitting (II)



For the third condition of a **non-negative row sum**, we compute

$$\sum_{L\in \mathrm{Neighbour}(K)} |F_{KL}| \left( D\frac{1-1}{d_{KL}} + U^{+}_{KL} - U^{-}_{KL} \right) = \sum_{L\in \mathrm{Neighbour}(K)} |F_{KL}| U_{KL}.$$

**This just means $\nabla_h \cdot \mathbf{U} = 0$ in the finite volume sense**.

The fourth condition is fulfilled due to appropriate boundary conditions.
$\Rightarrow$ **Convective-diffusive flux splitting yields a M-Matrix, if the flow field is divergence-free in the FVM-sense.** This result can be generalized to some nonlinear viscous conservation laws.

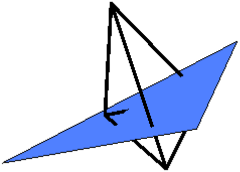
## Discrete Coupling between Fluid Flow and FVM (I)

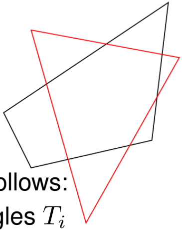
For the coupling of fluid flow and the FVM for a viscous conservation law, several possibilities exist.

**First approach**:

- use a $\mathbf{H}(\mathrm{div})$-conforming **AND** divergence-free FEM for an incompressible fluid (Darcy, Navier-Stokes equations, ...) and obtain a divergence-free velocity field $\mathbf{u}_h$;
  possible methods:
  Scott-Vogelius, divergence-free DG by Kanschat et al.
- compute in every time step an average velocity $U_{KL} = \frac{1}{|F_{KL}|} \int_{F_{KL}} \mathbf{u}_h \cdot \mathbf{n}_{KL}\, dS$ over each Voronoi face $F_{KL}$;
- associate the value $U_{KL}$ to the edge joining the control volumes $K$ and $L$; then a finite volume flow field is defined along all Delaunay edges which is divergence-free in the FVM sense;
- then the maximum principle holds for the discretized viscous conservation law

## Geometric Operations for the Coupling Procedure





The **algorithm for the coupling** in 3D works as follows:

- triangulate each Voronoi face $F_{KL}$ into triangles $T_i$
- extend each triangle $T_i$ to a plane $P_i$
- compute the cutting figure $Q$ between the plane $P_i$ and the neighboring tetrahedra (quadrangle)
- compute the cutting figure $H$ between $Q$ and $T_i$ (hexagon)
- triangulate the hexagon $H$
- using this triangulation, **compute exactly**

$$U_{KL} := \frac{1}{|F_{KL}|} \int_{F_{KL}} \mathbf{u}_h \cdot \mathbf{n} ds.$$

## Example: The Incompressible Navier-Stokes Equations in Strong Form

The **incompressible Navier-Stokes** equations:

$$\begin{aligned} \mathbf{u}_t - \frac{1}{\mathrm{Re}}\Delta\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p &= \mathbf{f}, && \text{in } \Omega \\ -\nabla\cdot\mathbf{u} &= 0 && \text{in } \Omega, \\ \mathbf{u} &= 0 && \text{on } \partial\Omega. \end{aligned}$$

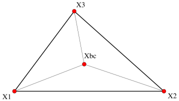
This nonlinear partial differential equation describes the time evolution of the velocity field $\mathbf{u}(\mathbf{x}, t)$ within the domain $\Omega$.

## Example: The Scott-Vogelius FEM for the Incompressible Navier-Stokes Equations

For a **conforming Galerkin mixed FEM discretization** we choose discrete spaces $\mathbf{V}_h \subset H_0^1(\Omega)^d$ and $Q_h \subset L_{2,0}(\Omega)$ and pose the following discrete problem: We look for $(\mathbf{u}_h, p_h)$, with $\mathbf{u}_h \in \mathbf{V}_h$, $p_h \in Q_h$,

$$(\partial_t \mathbf{u}_h, \mathbf{v}_h) + \frac{1}{\mathrm{Re}}(\nabla \mathbf{u}_h, \nabla \mathbf{v}_h) + (\mathbf{u} \cdot \nabla \mathbf{u}_h, \mathbf{v}_h) - (p_h, \nabla \cdot \mathbf{v}_h) - (\nabla \cdot \mathbf{u}_h, q_h) = (\mathbf{f}, \mathbf{v}_h),$$

for all test functions $\mathbf{v}_h \in \mathbf{V}_h$, $q_h \in Q_h$.
On shape regular and locally quasi-uniform **macro element meshes** for (d=2, 3), we use $V_h = (P_d)^d$ and $Q_h = P_{d-1}^{\mathrm{disc}}$, the classical **Scott-Vogelius** element.




The Scott-Vogelius element is **LBB-stable on macro element meshes** and **divergence-free** (testing by $\mathbf{v}_h = \mathbf{0}$, and $q_h = \nabla \cdot \mathbf{u}_h$)!

## Discrete Coupling between Fluid Flow and FVM (II)

**But the use of divergence-free FE methods is expensive.**
**Second approach**:

- **use a non-divergence-free FEM** for the incompressible fluid flow (Darcy, Navier-Stokes, ...) and compute a finite volume flow field $U_{KL}$ along the Delaunay edges as above;
- in the FVM discretization for the elliptic operator $-\nabla \cdot (D\nabla c - c\mathbf{u})$ **subtract a discretized term** $c\nabla \cdot \mathbf{u}$;
- then a discretization for $-D\Delta c + \mathbf{u} \cdot \nabla c$ arises, and the discrete maximum principle holds at least for a simple upwinding of the convection term, as shown above

## Discrete Coupling between Fluid Flow and FVM (III)

Use of divergence-free FE methods is expensive.

**Third approach**:

- use a non-divergence-free FE method in order to obtain an incompressible fluid (Darcy, Navier-Stokes, . . . ) and apply a discrete $L^2$ or a discrete $H^1$ projection onto the Delaunay grid (depending on the boundary conditions), in order to obtain a discretely divergence-free velocity field along the Delaunay edges
- idea: use a Darcy-like equation for the $L^2$ projection, resp., a Stokes-like equation for the $H^1$ projection:

$$\begin{aligned} \mathbf{v} + \nabla\phi &= \mathbf{u} \\ -\nabla\cdot\mathbf{v} &= 0; \end{aligned}$$

- assuming appropriate boundary conditions, we obtain

$$\begin{aligned} (\nabla\phi, \nabla\psi) &= (\mathbf{u}, \nabla\psi), \\ \mathbf{v} &= \mathbf{u} - \nabla\phi. \end{aligned}$$

- **The projection only needs integration along Delaunay edges!**

## Discrete Coupling between Fluid Flow and FVM (IV)

Design a finite volume method resp. covolume method for incompressible fluids on Delaunay meshes such that the natural FVM condition for mass conservation

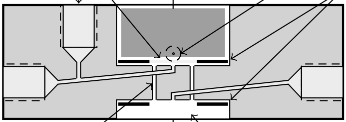
$$\sum_{L \in \mathrm{Neighbour}(K)} |F_{KL}| U_{KL} = 0$$

is fulfilled on every control volume $K$.

**A natural formulation would yield velocitites which are given along Delaunay edges.**
There is an appropriate approach for **Darcy's law in the case of an isotropic permeability tensor**, by solving a potential equation. The velocity field can be obtained through the gradient of the potential along the Delaunay edges.

**But what about the Stokes and Navier-Stokes equations, and coupled incompressible fluids?** Can we derive a method with velocity variables along the Delaunay edges?
**For the Stokes equations the answer is positive**, but for the Navier-Stokes equations the convection term makes some trouble. $\Rightarrow$ In the case of the Navier-Stokes equations use, e.g., a collocated scheme with pressure stabilization!

## An Application from Electrochemistry —- Electrochemical Flow Cells



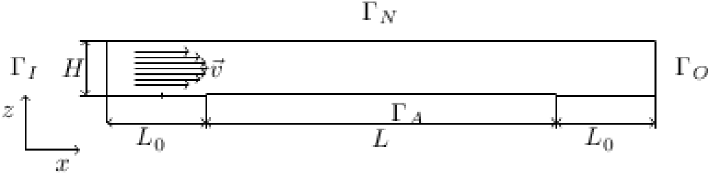

Differential electrochemical mass spectroscopy (**DEMS**) is a tool to gain information on **catalytic reactions in fuel cell** catalytic layers.

Classically, theoretical interpretations of electrochemical experiments are based on **asymptotic analysis** for **special experimental situations**, where PDE models in 1D or 2D are valid.

**Remarks**:

- ▷ Experimental devices used in practice often differ from the **model devices**
- ▷ **3D models** for the experiments based on PDEs are **rarely used** by electrochemists

## A Calibration Experiment — the Limiting Current




**Hydrogen** $H_2$ is dissolved in **dilute sulphuric acid** $H_2SO_4$. An **electrode reaction** takes place at a **platinum** $Pt$ electrode

$$H_2 \rightarrow 2H^+ + 2e^-.$$

At the electrode, the electrons $e^-$ enter an **external circuit** and recombine with the protons $H^+$ at a counter electrode outside of the domain of consideration.

The *Limiting Current* experiment clears up for a given experimental device, **at which flow rates asymptotic flow behaviour** can be expected.

## The Electrochemical Model for the Limiting Current Experiment

**Model assumptions**:

- 3d stationary **incompressible Navier-Stokes** equation for fluid
- 3d stationary convection-diffusion equation for $H_2$ **concentration**
- **influence of density variations ignored** (dissolved species dilute)
- **infinitely fast** $H_2$ **oxidation** $\Rightarrow$ **homogeneous Dirichlet boundary condition** c=0 on electrode $S_E$

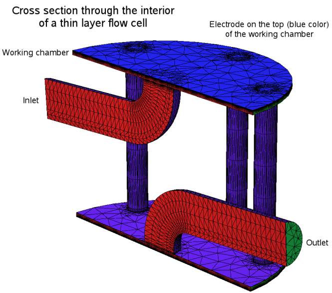
$$
\begin{aligned}
-\frac{1}{\mathrm{Re}}\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\,\mathbf{u} + \nabla p &= \mathbf{0} && \mathbf{x}\in\Omega \\
-\nabla\cdot\mathbf{u} &= 0 && \mathbf{x}\in\Omega \\
-\nabla\cdot(D\nabla c - c\mathbf{u}) &= 0 && \mathbf{x}\in\Omega
\end{aligned}
$$

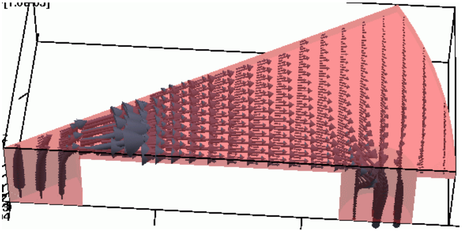
**Measured quantity**: **Anodic current**

$$
I_E = 2F\int_{S_E}(D\nabla c - c\mathbf{u})\cdot\mathbf{n}\,ds = 2F\int_{S_E} D\nabla c\cdot\mathbf{n}\,ds,
$$

with the Faraday constant $F$.

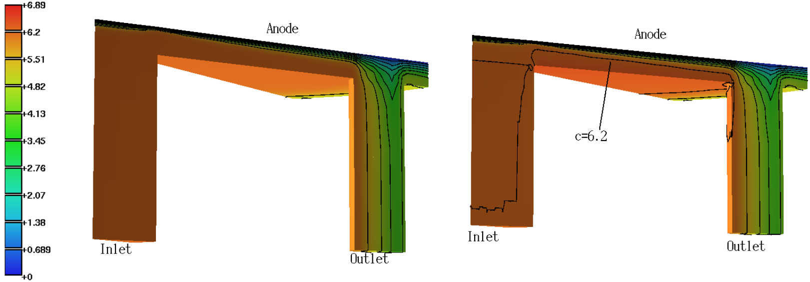
## Some Specifics Concerning the Simulation of the Jusys Flow Cell



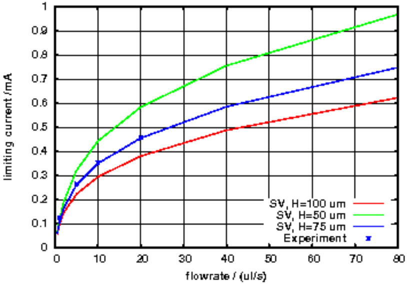
- reduction of the computational domain by **symmetry assumptions**
- **anisotropic, flow-aligned mesh** near to the electrode (parabolic boundary layer)
- adaptivity at the transition zones inlet - bulk domain, outlet - bulk domain
- **height of domain not exactly known** ($h \in [0.05, 0.1]\mathrm{mm}$)
- Reynolds number: experiments $[3, 60]$, simulation in $[1.4, 240]$
- Peclet number: experiments $[9.3 \cdot 10^2, 1.7 \cdot 10^4]$, simulation $[4.2 \cdot 10^2, 6.8 \cdot 10^4]$

## Qualitative Properties of the Numerical Results




**inlet concentration**: $6.2 \cdot 10^{-1} \mathrm{mol}/m^3$;
**color scale**: concentrations $\sim [0, 6.89 \cdot 10^{-1}]\,\mathrm{mol}/m^3$;
**FVM-Scott-Vogelius** fulfills **discrete maximum principle**
**FVM-Taylor-Hood violates** it;
Taylor-Hood: divergence-error at edge-singularity transported through the domain, see isoline $c = 6.2 \cdot 10^{-1}\,\mathrm{mol}/m^3$

## Comparison: Numerical Results & Experiment

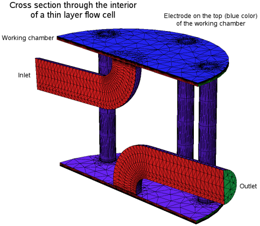



FVM-Scott-Vogelius **limiting current vs. flow rate**, assuming that height of the domain is $h \in \{0.05, 0.075, 0.1\}\mathrm{mm}$

$\Rightarrow$ **Calibration experiment reproduced well**, assuming that the height of the domain is $h = 0.075\mathrm{mm}$.

**Limiting current by Taylor-Hood** yields very similar results, probably since **functional is evaluated far away from singularities.**

# Outlook




- Implementation of coupling with discrete $L^2$ and $H^1$ projection;
- especially implementation of steady Stokes solver (generalization of MAC scheme);
- Implementation of a collocated solver for the incompressible Navier-Stokes equations within PDELIB (FEM-FVM ?)
- Applications