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Mass conservation of finite element methods for coupled flow-transport problems

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1. Introduction

Advection-diffusion equations arise in a number of important applications. Their robust and accurate numerical solution is – in case of advection dominated flows – still a challenge. Often it is neglected that the physical processes are governed by a velocity field u which itself is the solution of a hydrodynamical model like the incompressible Navier-Stokes equations. In this paper we address the issue of mass conservation when the underlying velocity field u in the transport equation is replaced by an approximation u_h.

We consider the simplest case of a coupled flow-transport problem in a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. The system is described by the instationary, incompressible Navier–Stokes equations

$$\begin{aligned} u_t - \nu\triangle u + (u\cdot\nabla)u + \nabla p &= f && \text{in } \Omega\times(0,T],\\ \operatorname{div} u &= 0 && \text{in } \Omega\times(0,T],\\ u &= u_b && \text{on } \partial\Omega\times(0,T],\\ u(0) &= u^0 && \text{in } \Omega, \end{aligned} \tag{1}$$

and the time-dependent transport equation

$$\begin{aligned} c_t - \varepsilon\triangle c + u\cdot\nabla c &= g && \text{in } \Omega\times(0,T],\\ (cu - \varepsilon\nabla c)\cdot n &= c_I\, u\cdot n && \text{on } \Gamma_-\times(0,T],\\ \varepsilon\nabla c\cdot n &= 0 && \text{on } \Gamma_+\times(0,T],\\ c(0) &= c^0 && \text{in } \Omega. \end{aligned} \tag{2}$$

Here, u and p denote the velocity and the pressure of the fluid, respectively, ν and ε are small positive numbers, $T > 0$ defines the final time. The boundary $\partial\Omega$ is splitted into the inflow boundary $\Gamma_- := \{x \in \partial\Omega : u\cdot n < 0\}$ and the outflow boundary $\Gamma_+ := \partial\Omega \setminus \Gamma_-$ where n is the unit outer normal. Furthermore, c is the concentration and c_I the concentration at the inflow boundary Γ_-. We assume that the given velocity field u_b on the boundary $\partial\Omega$ is the restriction of a divergence free function which we denote again by u_b. The initial velocity u^0 satisfies the incompressibility constraint $\nabla\cdot u^0 = 0$.

Different discretization methods for both the instationary, incompressible Navier–Stokes equations and the transport equation have been developed also in the practically important case of $\nu \ll 1$ and $\varepsilon \ll 1$, for an overview see [12]. We study the mass conservation of the discretized transport equation when using stabilized schemes. For simplicity of notation we restrict ourselves to the semidiscretization in time of the problems (1) and (2). The results can be extended to the fully discretized problems using the discontinuous Galerkin method in time.

2. Algorithms for the transport equation

2.1. Weak formulation and mass conservation

Let $W := H^1(\Omega)$, $(\cdot,\cdot)$ and $\langle\cdot,\cdot\rangle_\Gamma$ denote the L^2-inner products on Ω and Γ, respectively. A weak formulation of the transport problem (2) is given by

Find $c(t) \in W$ such that for all $\varphi \in W$: $(c(0) - c^0, \varphi) = 0$ and

$$\frac{d}{dt}(c,\varphi) + \varepsilon(\nabla c, \nabla\varphi) + (u\cdot\nabla c, \varphi) - \langle c\, u\cdot n, \varphi\rangle_{\Gamma_-} = (g,\varphi) - \langle c_I\, u\cdot n, \varphi\rangle_{\Gamma_-}. \tag{3}$$

Setting $\varphi = 1$ and using the incompressibility constraint $\nabla\cdot u = 0$, we get from (3) the global mass conservation property

$$\frac{d}{dt}\int_\Omega c\,dx + \int_{\Gamma_-} c_I\, u\cdot n\,d\gamma + \int_{\Gamma_+} c\, u\cdot n\,d\gamma = \int_\Omega g\,dx. \tag{4}$$

Let the domain Ω be polyhedral. We are given a family $\{\mathcal{T}_h\}_{h>0}$ of shape-regular triangulations of Ω into simplicial elements K. The diameter of K is denoted by h_K while $h := \max\{h_K : K \in \mathcal{T}_h\}$. Let $W_h \subset W$ be a finite element space for approximating the concentration. Then, the standard Galerkin discretization of (3) reads

Find $c_h(t) \in W_h$ such that for all $\varphi_h \in W_h$: $(c_h(0) - c^0, \varphi_h) = 0$ and

$$\frac{d}{dt}(c_h,\varphi_h) + \varepsilon(\nabla c_h, \nabla\varphi_h) + (u_h\cdot\nabla c_h, \varphi_h) - \langle c_h\, u_h\cdot n, \varphi_h\rangle_{\Gamma_-} = (g,\varphi_h) - \langle c_I\, u_h\cdot n, \varphi_h\rangle_{\Gamma_-} \tag{5}$$

where the solenoidal vector field u has been replaced by some – in general – discontinuous approximation u_h. Now setting $\varphi_h = 1$ and using elementwise integration by parts, we end up with

$$\frac{d}{dt}\int_\Omega c_h\,dx + \int_{\Gamma_-} c_I u_h\cdot n\,d\gamma + \int_{\Gamma_+} c_h u_h\cdot n\,d\gamma = \int_\Omega g\,dx + m_h(c_h,u_h) \tag{6}$$

where compared to the global mass conservation on the continuous level, see (4), the additional term

$$m_h(c_h,u_h) := \sum_{K\in\mathcal{T}_h}(c_h, \nabla\cdot u_h)_K + \sum_{E\in\mathcal{E}_h}\langle c_h, [u_h\cdot n_E]_E\rangle_E \tag{7}$$

is present. Here, $\mathcal{E}_h$ denotes the set of inner faces E, $(\cdot,\cdot)_K$ and $\langle\cdot,\cdot\rangle_E$ denote the L^2-inner products on K and E, respectively. With each $E \in \mathcal{E}_h$ we associate an arbitrary but fixed unit normal n_E and define the jump of ψ across the common face E of the two adjacent elements K and $\widetilde{K}$ by

$$[\psi]_E := u_h|_{\widetilde{K}}\Big|_E - u_h|_K\Big|_E$$

where n_E is an outer normal to K. Conditions which guarantee that $m_h = 0$ will be discussed in the following Sections.

2.2. Stabilized schemes for the transport equation

In the case that $0 < \varepsilon \ll 1$, the standard Galerkin discretization exhibits spurious oscillations which can be suppressed by using some sort of stabilized schemes. We consider stabilized schemes of the following type:

Find $c_h(t) \in W_h$ such that for all $\varphi_h \in W_h$: $(c_h(0) - c^0, \varphi_h) = 0$ and

$$\begin{aligned}\frac{d}{dt}(c_h,\varphi_h) + \varepsilon(\nabla c_h, \nabla\varphi_h) + (u_h\cdot\nabla c_h, \varphi_h) - \langle c_h\, u_h\cdot n, \varphi_h\rangle_{\Gamma_-} \\ + S_h(c_h,\varphi_h) = (g,\varphi_h) - \langle c_I\, u_h\cdot n, \varphi_h\rangle_{\Gamma_-}.\end{aligned} \tag{8}$$

In the Streamline Diffusion (SD) method [2] we add weighted residuals of the strong form of the differential equation. Thus, we have

$$S_{sd}(c_h, \varphi_h) := \sum_{K \in \mathcal{T}_h} \tau_K (c_{h,t} - \varepsilon \triangle c_h + u_h \cdot \nabla c_h - g, u_h \cdot \nabla \varphi_h)_K \tag{9}$$

with a user-chosen parameter τ_K.

In the subgrid scale method [6, 10], the space W_h contains a subspace of resolvable scales $W_H \subset W_h$ which is given by a projector $P_H : W_h \to W_H$. Then, the non-resolvable scales are stabilized by adding

$$S_{subg}(c_h, \varphi_h) := \sum_{K \in \mathcal{T}_h} \tau_K (\nabla (id - P_H) c_h, \nabla (id - P_H) \varphi_h)_K \tag{10}$$

to the standard Galerkin approach (5).

Finally, we mention the stabilization by local projection [1] which relies on a local projection operator $\widetilde{P} : W_h \to D_h$ into a proper space of discontinuous finite elements. Here, the added stabilizing term becomes

$$S_{locp}(c_h, \varphi_h) := \sum_{K \in \mathcal{T}_h} \tau_K \big((id - \widetilde{P}) \nabla c_h, (id - \widetilde{P}) \nabla \varphi_h \big)_K. \tag{11}$$

Note that in the subgrid scale method the unresolvable scales are stabilized by an artificial viscosity term whereas in the local projection method the fluctuations of the gradients, i.e., $(id - \widetilde{P}) \nabla c_h$, are controlled in the L^2-norm.

With respect to our purpose we see that in all considered cases the stabilizing terms vanish for $\varphi_h = 1$. Thus, the global mass conservation will be guaranteed provided that the additional term $m_h(c_h, u_h)$ in (6) vanishes.

3. Algorithms for the incompressible Navier–Stokes equations

3.1. Weak formulation and Galerkin approach

Let $V := H_0^1(\Omega)^d$, $M := L^2(\Omega)$, and $Q := \big\{ q \in M : (q, 1) = 0 \big\}$. A weak formulation of the Navier–Stokes problem (1) which is obtained in a standard way reads

Find $\big(u(t), p(t)\big) \in (u_b + V) \times Q$ such that for all $v \in V:\ (u(0) - u^0, v) = 0$ and

$$\frac{d}{dt}(u, v) + \nu (\nabla u, \nabla v) + \big((u \cdot \nabla) u, v \big) - (\nabla \cdot v, p) = (f, v) \qquad \forall v \in V, \tag{12}$$

$$(\nabla \cdot u, q) = 0 \qquad \forall q \in Q. \tag{13}$$

Our assumption that u_b is the restriction of a divergence free function yields

$$(\nabla \cdot u, 1) = \langle u \cdot n, 1 \rangle_{\partial\Omega} = \langle u_b \cdot n, 1 \rangle_{\partial\Omega} = (\nabla \cdot u_b, 1) = 0. \tag{14}$$

This combined with (13) implies that $(\nabla \cdot u, q) = 0$ for all $q \in L^2(\Omega)$.

We consider inf-sup stable discretizations of the problem (12), (13). Let $V_h \subset V$, $M_h \subset M$, and $Q_h = M_h \cap Q$ be finite element spaces such that the inf-sup condition

$$\inf_{q_h \in Q_h} \sup_{v_h \in V_h} \frac{(\nabla \cdot v_h, q_h)}{|v_h|_1 \, \|q_h\|_0} \geq \beta \tag{15}$$

is satisfied with a positive constant β which is independent of the mesh size parameter h. Using the discrete spaces V_h and M_h, the standard Galerkin approach of (12), (13) reads

Find $\big(u_h(t), p_h(t)\big) \in (u_{b,h} + V_h) \times M_h$ such that for all $v_h \in V_h :\ (u_h(0) - u^0, v_h) = 0$ and

$$\frac{d}{dt}(u_h, v_h) + \nu(\nabla u_h, \nabla v_h) + \big((u_h \cdot \nabla)u_h, v_h\big) - (\nabla \cdot v_h, p_h) = (f, v_h) \qquad \forall v_h \in V_h, \qquad (16)$$

$$(\nabla \cdot u_h, q_h) = 0 \qquad \forall q_h \in Q_h, \qquad (17)$$

where $u_{b,h}$ is a suitable approximation of u_b which satisfies the condition $\langle u_{b,h} \cdot n, 1\rangle_{\partial\Omega} = 0$. As a consequence

$$(\nabla \cdot u_h, 1) = \sum_{K\in\mathcal{T}_h} (\nabla \cdot u_h, 1)_K = \langle u_{b,h} \cdot n, 1\rangle_{\partial\Omega} - \sum_{E\in\mathcal{E}_h} \langle [u_h]_E \cdot n_E, 1\rangle_E = -\sum_{E\in\mathcal{E}_h} \langle [u_h]_E \cdot n_E, 1\rangle_E.$$

Thus, if the normal components of u_h are continuous over the faces we get the discrete analogon of (14), i.e., $(\nabla \cdot u_h, q_h) = 0$ for all $q_h \in M$.

While discretizing the Navier–Stokes problem by inf-sup stable finite elements, one has to make the fundamental decision of choosing either a continuous or discontinuous pressure approximation. Due to (17), the incompressibility constraint $\nabla \cdot u = 0$ from (1) is fulfilled only in an approximate sense. If discontinuous pressure approximations are used, the mass conservation is satisfied more locally since functions with support within one element can be used as test functions.

3.2. Stabilized schemes for the Navier-Stokes equations

In recent years, a huge number of schemes have been developed to stabilize both the effect of dominating advection and the instabilities caused by using finite element pair V_h and Q_h which do not satisfy (15), see e.g. [1, 11, 14]. In particular, the use of equal order interpolation of velocity and pressure with the streamline diffusion method or the stabilization by local projection seems to be quite popular. However, a common feature of these types of stabilization methods is an additional 'stabilizing' term in the mass balance (13) of the Navier-Stokes equation which produces an additional error for the mass conservation of the transport equation (6). For avoiding this additional discretization error, one should try to separate the stabilization of the two instability phenomena: dominating advection and use of unstable finite element pairs for approximating velocity and pressure. Such a separation technique has been considered e.g. in [3, 7, 8].

In the following we want to restrict ourselves to the solution of the Navier-Stokes equations by inf-sup stable conforming finite element pairs. In this case, the computed velocity field $u_h(t) \in u_{b,h} + V_h$ belongs to $H^1(\Omega)^d$ and is discretely divergence free in the sense that

$$(\nabla \cdot u_h, q_h) = 0 \qquad \forall q_h \in M_h.$$

Note that (17) implies that this relation holds first for all $q_h \in Q_h \subset M_h$ but the choice of the approximation $u_{b,h}$ of the boundary data u_b indeed guarantees its fulfillness for all $q_h \in M_h$.

4. Mass conservative methods

We have seen in Section 2. that the mass conservation on the discrete level is guaranteed when the term $m_h(c_h, u_h)$ vanishes. On the continuous level the term $m_h(c_h, u)$ vanishes due to incompressibility condition $\nabla \cdot u = 0$ and $[u \cdot n_E]_E = 0$ for all inner faces. In the following subsections, we will discuss several possibilities which ensure $m_h(c_h, u_h) = 0$.

4.1. Higher-order approximation of the flow problem

Let us assume that the transport equation will be solved by a method of order $r \geq 1$, i.e., the approximation error in space will satisfy

$$\inf_{\varphi\in W_h} |c - \varphi_h|_m \leq C\, h^{r+1-m}|c|_{r+1}, \qquad c \in H^{r+1}(\Omega),\ 0 \leq m \leq r+1.$$

One could think for example to use continuous, piecewise polynomials of degree less than or equal to r. In the following, we will shortly note this space by P_r. We observe that $m_h(c_h, u_h)$ vanishes if $c_h \in M_h$, in particular if $W_h \subset M_h$. Thus, in the considered case we could choose the space P_r to be a subspace of pressure space M_h. This means that the pressure will be approximated in the L^2-norm of order $r+1$. In order to ensure the inf-sup condition the velocity has to be approximated by suitable elements of order $r+1$ like P_{r+1}. We end up with the following discretization for $(u_h, p_h, c_h) \in P_{r+1} \times P_r \times P_r$. Hence, the Navier–Stokes problem has to be discretized by a method which is one order better than the method used for the transport equation. Note that this technique works for both, continuous and discontinuous pressure approximations.

A similar statement is also true for nonconforming finite element discretizations of the Navier-Stokes equations since a nonconforming discretization for the velocities of order $r+1$ is assumed to satisfy

$$\langle [u_h]_E, r_h \rangle_E = 0 \qquad \forall r_h \in P_r(E),\ \forall E \in \mathcal{E}_h.$$

If the discretization is completed by elements of order r for the approximation of pressure and concentration, then we conclude from (7) that $m_h(c_h, u_h) = 0$. Thus, again a one order higher discretization of the flow problem results in a mass conservation of the transport problem.

However, from the practical point of view, this technique seems to be non-attractive since the discretization of the Navier–Stokes problem by a higher order method is too costly.

4.2. Post-processing of the discrete velocity

Another idea for ensuring the exact mass balance on the discrete level consists in replacing the discrete velocity solution u_h by a different discrete function w_h which is close to u_h. This technique was proposed in [4] for the local discontinuous Galerkin method applied to flow problems. To be precise, instead of solving the standard weak formulation of the transport equation, see (5), the following problems will be solved

Find $c_h(t) \in W_h$ such that for all $\varphi_h \in W_h$: $\quad (c_h(0) - c^0, \varphi_h) = 0$ and

$$\frac{d}{dt}(c_h, \varphi_h) + \varepsilon(\nabla c_h, \nabla \varphi_h) + (w_h \cdot \nabla c_h, \varphi_h) - \langle c_h\, w_h \cdot n, \varphi_h \rangle_{\Gamma_-} = (g, \varphi_h) - \langle c_I\, w_h \cdot n, \varphi_h \rangle_{\Gamma_-} \quad (18)$$

Let the Navier–Stokes equations be discretized by the inf-sup stable finite element pair $P_r^{\text{bubble}}/P_{r-1}^{disc}$ consisting of the velocity space of continuous, piecewise polynomials of degree r enriched with certain bubble function and the pressure space of discontinuous, piecewise polynomials of degree $r-1$, [9]. We will construct the function w_h which acts as the velocity field in the transport equation by a post-processing. To this end, we define on each element $K \in \mathcal{T}_h$ the vector-valued local interpolation operator $P_K : H^1(K)^d \to P_r(K)^d$ by

$$\big\langle (P_K v) \cdot n_K, \varphi \big\rangle_E = \langle v \cdot n_K, \varphi \rangle_E \qquad \forall E \subset \partial K,\ \varphi \in P_r(E), \quad (19)$$

$$(P_K v, \nabla \varphi) = (v, \nabla \varphi) \qquad \forall \varphi \in P_{r-1}(K), \quad (20)$$

$$(P_K v, \psi) = (v, \psi) \qquad \forall \psi \in \Psi_r(K), \quad (21)$$

where

$$\Psi_r(K) := \big\{ \psi \in L^2(K)^d \ :\ (DF_K^T \psi) \circ F_K \in \widehat{\Psi}_r \big\}$$

with

$$\widehat{\Psi}_r := \big\{ \hat\psi \in P_r(\widehat{K})^d \ :\ \nabla \cdot \hat\psi = 0 \text{ in } \widehat{K},\ \hat\psi \cdot n_{\widehat{K}} = 0 \text{ on } \partial \widehat{K} \big\}.$$

In the above formulas we have used the reference transformation $F_K : \widehat{K} \to K$ which is a bijective mapping from the reference cell $\widehat{K}$ onto the original cell K. Further, $\hat\psi = \psi \circ F_K$. The definition of P_K by (19)-(21) is the customization of the interpolation operator $\mathbb{P}$ which was introduced in [4] in the frame of local discontinuous Galerkin methods. The local interpolation operators P_K can be put together to a global interpolation operator P_h in the following way

$$(P_h v)|_K := P_K(v_h|_K).$$

Note that, in general, the function $P_h v$ will not belong to $H^1(\Omega)^d$.

Next we will show that the post-processed solution $P_h u_h$ is piecewise divergence free. We start with the incompressibility constraint (17) and use the conditions (19) and (20) of the definition of P_K to obtain

$$\begin{aligned} 0 = (\nabla \cdot u_h, q_h)_K &= -(u_h, \nabla q_h)_K + \langle u_h \cdot n_K, q_h \rangle_{\partial K} \\ &= -(P_K u_h, \nabla q_h)_K + \langle (P_K u_h) \cdot n_K, q_h \rangle_{\partial K} = (\nabla \cdot P_K u_h, q_h)_K. \end{aligned}$$

Here, we have used $\nabla q_h \in P_{r-1}(K)^d$ and $q_h|_E \in P_r(E)$ for all faces $E \subset \partial K$.

Furthermore, we notice that the function α which is piecewise defined by

$$\alpha|_K := \nabla \cdot P_K u_h$$

belongs to Q_h. Since $\alpha_K \in P_{r-1}(K)$ holds true, we have to show only that α has zero integral mean over Ω. Indeed, we get

$$\int_\Omega \alpha \, dx = \sum_{K \in \mathcal{T}_h} \int_K \nabla \cdot P_K u_h \, dx = \sum_{K \in \mathcal{T}_h} \int_{\partial K} (P_K u_h) \cdot n_K \, d\gamma = \sum_{K \in \mathcal{T}_h} u_h \cdot n_K \, d\gamma = \int_{\partial\Omega} u_h \cdot n \, d\gamma = 0,$$

where we have used the condition (19).

Hence, α can be used as a pressure test function in (17). Using this, we obtain

$$0 = (\nabla \cdot P_h u_h, \alpha) = \sum_{K \in \mathcal{T}_h} (\nabla \cdot P_h u_h, \nabla \cdot P_h u_h)_K$$

which gives $\nabla \cdot P_h u_h|_K \equiv 0$, i.e., the post-processed velocity solution is piecewise divergence free.

The modified convection field in (18) is chosen to be $w_h := P_u u_h$. This ensures that the first term of $m_h(c_h, w_h)$ vanishes. Moreover, the normal component of w_h has no jumps across inner faces due to condition (19) in the definition of P_K. Indeed, we have for all $\varphi \in P_r(E)$ that

$$\big\langle [P_h u_h]_E \cdot n_E, \varphi \big\rangle_E = \langle P_{\widetilde{K}} u_h \cdot n_E, \varphi \rangle_E - \langle P_K u_h \cdot n_E, \varphi \rangle_E = \langle u_h \cdot n_E, \varphi \rangle_E - \langle u_h \cdot n_E, \varphi \rangle_E = 0$$

where K and $\widetilde{K}$ are the two elements which are adjacent to E. Since $[P_h u_h]_E \in P_r(E)$ holds true, we conclude $[P_h u_h]_E = 0$. Hence, also the second term of $m_h(c_h, w_h)$ vanishes.

Compared to the method of Section 4.1., we solve both the transport and the Navier-Stokes equation with a method of order r. Nevertheless, the mass conservation on the discrete level is guaranteed.

4.3. Scott-Vogelius elements

Now, we will concentrate on finite element discretizations which guarantee that the discrete velocity solution u_h is piecewise divergence free. To this end, let us consider discretizations with $P_r/P_{r-1}^{\text{disc}}$-elements. It is well-known that in the two-dimensional case for $r \geq 4$, this finite element pair is inf-sup stable when special meshes which exhibit so called singular vertices, are excluded, see [13]. Furthermore, it has been shown recently that there are macroelement meshes in two and three dimensions on which this pair of finite elements is inf-sup stable [15] provided that the polynomial degree r is greater than or equal to the space dimension d. Although a restriction on the mesh is needed this pair is attractive since a discretely divergence free function is piecewise divergence free. Indeed, due to the participating discrete spaces, the divergence of each discrete velocity field belongs to the pressure space. Hence, the weak compressibility condition (17) yields

$$0 = (\nabla \cdot u_h, \nabla \cdot u_h),$$

i.e., the discrete velocity solution u_h is divergence free in the L^2-sense. Of course, this results in $m_h(c_h, u_h) = 0$ since the continuous velocity approximation u_h has no jumps.

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