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A Variational Solution to the Transport Equation Subject to an Affine Constraint

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Abstract

We establish an existence and uniqueness theorem for the transport equation subject to an inequality affine constraint, viewed as a constrained optimization problem. Then we derive a Space-Time Integrated Least Squares (STILS) scheme for its numerical approximation. Furthermore, we discuss some L^2-projection strategies and with numerical examples we show that there are not relevant for that problem.

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A Variational Solution to the Transport Equation Subject to an Affine Constraint

1 Introduction

1.1 Context

In numerous problems, *e.g.*, low MACH number flows [10] or reacting flows in porous media [3], the density ρ, for a given velocity u, obeys the transport equation subject to an equality affine constraint:

$$\left\{\begin{array}{rcl} \partial_t \rho & = & f - \mathrm{div}(\rho u) \\ 0 & = & a\rho + b \end{array}\right. \tag{TCE}$$

where f, a and b are regular functions; *e.g.*, in the context of low MACH number flows, $f = 0$, $a = RT$ and $b = -p_0$.

Since the constraint of (TCE) is in general not an invariant of the PDE, the very notion of solution to the problem is ambiguous. In the context of ODEs, similar problems have been treated as differential-algebraic equations [9]. In fact, frequently, the constraint in (TCE) arises from asymptotic developments, *i.e.*, higher order terms have been dropped and one could just as well consider an inequality constraint. In addition, numerically, the constraint enforcement is necessarily approximate. Therefore, we rather consider

$$\left\{\begin{array}{rcl} \partial_t \rho & = & f - \mathrm{div}(\rho u) \\ -\varepsilon_1 & \leq & a\rho + b \leq \varepsilon_2 \end{array}\right. \tag{TC}$$

where f, a, b, ε_1 and ε_2 are given regular functions, the latter two being non negative.

1.2 Motivation

Let us show with a one sided inequality: $0 \leq \rho + b$ and a simple 1-dimensional example with a divergence free velocity u that an L^2 projection strategy is not equivalent to solving the associated variational inequality.

1.2.1 Method of Characteristics with Projection

A method of characteristics, in an L^2 setting for the Transport Equation involves solving $\frac{\partial x(t,X_0)}{\partial t} = u(x(t,X_0),t)$ with the notation $x(0,X_0) = X_0$, then computing the jacobian $J(X_0,t) = |\det \frac{\partial x}{\partial X_0}|$ (which can be seen as representing volume dilatation due to the change of variables $(x,t) \mapsto (X_0,t)$). A weak solution of the Transport equation then reads ([11] appendix C6):

$$(X_0,t) \mapsto \rho(x(t,X_0),t) = \left(\rho(X_0,0) + \int_0^t f(x(s,X_0),s)\,\mathrm{d}s\right) \times J(X_0,t), \qquad \text{(wsT)}$$

and the L^2-projected solution on the constraint subset is:

$$\rho_{\mathrm{pr}}(x,t) = \left(\rho(x,t) + b(t)\right)^+ - b(t) \qquad \text{(wsTp)}$$

where z^+ denotes the positive part of z.

Example 1.1. Consider the case $f : t \mapsto t^2 - t$, $b : t \mapsto -0.8t$ and $\rho_0 = 1/12$. Then, $\frac{\partial x(t,X_0)}{\partial t} = 0$, and thus (wsT) becomes:

$$(X_0,t) \mapsto \rho(x(t,X_0),t) = \left(\frac{1}{12} + \frac{t^3}{3} - \frac{t^2}{2}\right) \times 1,$$

and the corresponding ρ_{pr} is deduced from (wsTp). These particular solutions ρ and ρ_{pr} are depicted in Figure 1, left and center frames.

1.2.2 Variational Inequality Approach

Now if we consider the variational inequality associated with the constraint $0 \le \rho + b$, with $u = 0$, we have (see [6] p. 76 remark 3.9):

$$\begin{cases} \partial_t \rho_{\mathrm{iv}} &= b' + (f - b')^+ - \mathrm{sgn}^+(\rho_{\mathrm{iv}} + b(t))(f - b')^- \\ \rho_{\mathrm{iv}}(0) &= \rho_0 \end{cases}$$

where $\mathrm{sgn}^+(z)$ is one if z is positive and zero otherwise.

Example 1.2. With the same hypothesis as in Example 1.1, the solutions ρ_{iv} is computed using this modified right-hand side, and is shown in Figure 1, right frame.

Clearly, the above examples show that projection and variational inequality approaches can lead to different solutions. The solution to the variational inequality can be considered

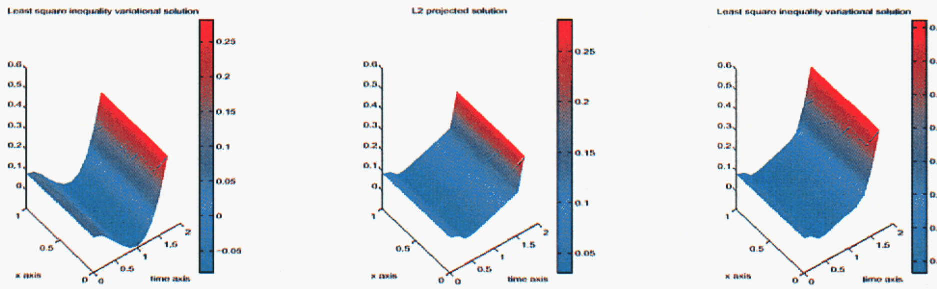

Figure 1. Solutions of Example 1.1: without constraint (left), L^2-projected (center), and variational inequality (right).

as a global time projection method useful in the context of multi-time stepping and parallel computing. It is not reduced to a simple L^2 projection at final time. The Least Square formulation for the Transport equation as been demonstrated to be an efficient method for irregular velocity [1], therefore it is promising to extend it to the Transport Equation subject to a constraint.

1.3 Outline

Considering (TC) under acceptable conditions, we prove it is a well-posed constrained optimization problem in the context of least square formulations of the Transport equation. The solution obtained is shown to be the same as the one yielded by the variational inequality. We then consider a mixed formulation and establish that it leads to the same solution, from which we finally derive a simple space-time finite element method, STILS, to approximate this solution. Note that, in [4], a similar approach is used for a 1D conservation law with unilateral constraint treated with a projection-penalization strategy in the context of entropy formulations.

2 Functional Setting

Defining Q by $Q = [0, t_f] \times \Omega$, where Ω is a domain of $\mathbb{R}^3$, and ∂Q_- as the part of the boundary of Q where $\langle u|n \rangle < 0$, and denoting n as the outward normal vector on the boundary of Q, (TC) becomes:

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho u) &= f \quad \text{in } Q \\ -\varepsilon_1 \leq a\rho + b &\leq \varepsilon_2 \quad \text{in } Q \\ \rho &= \rho_e \quad \text{in } \partial Q_- \end{cases} \tag{TCbc}$$

and we will henceforth assume $a \in \mathrm{L}^\infty(Q)$, $(b, \varepsilon_1, \varepsilon_2) \in \mathrm{L}^2(Q)^3$. The problem is formalized accordingly:

Defi nition 2.1. For $u \in \mathrm{L}^\infty([0,t_f], (\mathrm{H}^1(\Omega) \cap \mathrm{L}^\infty(\Omega))^3)$ such that $\operatorname{div} u \in \mathrm{L}^1([0,t_f], \mathrm{L}^\infty(\Omega))$, define the unbounded operator $\mathcal{D}\cdot = \partial_t \cdot + \operatorname{div}(u\cdot)$ over $\mathrm{L}^2(Q)$ (identified with $\mathrm{L}^2([0,t_f], \mathrm{L}^2(\Omega))$) and the BANACH space $V(u,Q) = \{\varphi \in \mathrm{L}^2(Q) : \mathcal{D}\varphi \in \mathrm{L}^2(Q)\}$ equipped with the graph norm

$$\|\varphi\|^2 = \int_Q (\mathcal{D}\varphi)^2 \,\mathrm{d}t\mathrm{d}x + \int_Q \varphi^2 \,\mathrm{d}t\mathrm{d}x.$$

The subspace $V_0(u,Q) = \{\varphi \in V(u,Q) : \varphi_{|\partial Q_-} = 0\}$, where the trace $\varphi_{|\partial Q_-}$ is to be understood in a weak sense, is equipped with the seminorm

$$|\varphi|_{1,\operatorname{div} u} = \left(\int_Q (\mathcal{D}\varphi)^2 \,\mathrm{d}t\mathrm{d}x \right)^{\frac{1}{2}}.$$

In all which follows, the hypothesis of Definition 2.1 regarding the regularity of u and $\operatorname{div} u$ will be assumed to hold. It is in particular proved in [5] that $|\cdot|_{1,\operatorname{div} u}$ is a norm equivalent to the graph norm on $V_0(u,Q)$. By extending the boundary condition ρ_e in $\widetilde{\rho}_e$ on Q, and by defining $c = \rho - \widetilde{\rho}_e$, (TCbc) becomes:

$$\begin{cases} \mathcal{D}c &= f \quad \text{in } Q \\ -\varepsilon_1 \leq g(c) &\leq \varepsilon_2 \quad \text{in } Q \end{cases} \tag{TCh}$$

where g is the affine operator $\mathrm{L}^2(Q) \to \mathrm{L}^2(Q)$ defined by $\varphi \mapsto a\varphi + b + a\widetilde{\rho}_e$.

3 The Constrained Optimization Point of View

The set $K = \{q \in \mathrm{L}^2(Q), -\varepsilon_1 \leq g(q) \leq \varepsilon_2\}$ is convex by definition of g, and its indicator function (equal to 0 on K, $+\infty$ elsewhere) is convex lower semicontinuous, *cf.* Lemma 2.8.2 in [6]. Define

$$\begin{array}{rccl} J: & V_0(u,Q) & \longrightarrow & [0, +\infty] \\ & \varphi & \longmapsto & \frac{1}{2}\|\mathcal{D}\varphi - f\|^2_{\mathrm{L}^2(Q)} + I_K(\varphi) \end{array}$$

which is convex, lower semicontinuous and 0-coercive. We thus have (*cf.* Proposition 1.2 in [8]):

Lemma 3.1. *There exists a unique $c = \mathrm{Argmin}_{\varphi \in V_0(u,Q)} J(\varphi)$. In addition, $c \in K$.*

Now, the domain of J is $K \cap V_0(u,Q)$ and, denoting by $\partial J(q)$ its subdifferential at any $q \in K \cap V_0(u,Q)$, $c = \mathrm{Argmin}_{\varphi \in V_0(u,Q)} J(\varphi)$ is characterized by

$$0 \in \partial J(c) \iff -\mathcal{D}^*(\mathcal{D}c - f) \in \partial I_K(c) \tag{1}$$

$$\iff (\forall \varphi \in K \cap V_0(u,Q))\ \langle \mathcal{D}^*(\mathcal{D}c - f) | (\varphi - c) \rangle_{\mathrm{L}^2(Q)} \geq 0 \tag{2}$$

which in other words means that c is a fixed point: $c = \Pi_K(c + \mathcal{D}^* f - \mathcal{D}^* \mathcal{D}c)$, where Π_K is the L^2 projector onto K.

Remark 3.2. According to [5], $\mathcal{D}$ is bijective, and thus we have:

$$(\forall \varphi \in K \cap V_0(u,Q)))\quad \left\langle \mathcal{D}(c - \mathcal{D}^{-1} f) | \mathcal{D}(\varphi - c) \right\rangle_{\mathrm{L}^2(Q)} \geq 0$$

whence $c = \Pi_K^{\mathcal{D}}(\mathcal{D}^{-1} f)$, where $\Pi_K^{\mathcal{D}}$ denotes the projector from $V_0(u,Q)$ onto K for $\langle \mathcal{D} \cdot | \mathcal{D} \cdot \rangle_{\mathrm{L}^2(Q)}$.

Remark 3.3. In the case where K is the convex cone of nonnegative functions, let $\overline{c} \in V_0(u,Q)$ be the solution of $\mathcal{D}\overline{c} = f^+ - \mathrm{sgn}^+(\overline{c}) f^-$, then $\overline{c} \in K$ and satisfies:

$$(\forall \varphi \in K)\quad \langle f - \mathcal{D}\overline{c} | \varphi - \overline{c} \rangle_{\mathrm{L}^2(Q)} \leq 0.$$

From [5] we know that

$$(\forall \theta \in K)\ (\exists \psi \in K \cap V_0(u,Q))\quad \mathcal{D}\psi = \theta,$$

and we deduce that

$$(\forall \psi \in K \cap V_0(u,Q))\quad \langle f - \mathcal{D}\overline{c} | \mathcal{D}\psi \rangle_{\mathrm{L}^2(Q)} \leq 0.$$

Since $\langle f - \mathcal{D}\overline{c} | \mathcal{D}\overline{c} \rangle_{\mathrm{L}^2(Q)} \geq 0$, we conclude that $\overline{c}$ is the solution of the constrained optimization problem $\mathrm{Min}_{\varphi \in V_0(u,Q)} J(\varphi)$.

4 Mixed Formulation

Since g is affine, it has an associated linear operator G allowing a mixed formulation of (TCh) as follows: with $\Lambda = \{\lambda \in \mathrm{L}^2(Q), \lambda \geq 0\}$, find $(c, \lambda_1, \lambda_2) \in V_0(u,Q) \times \mathrm{L}^2(Q)^2$ such that

$$\begin{cases} (\forall \varphi \in V_0(u,Q)) & \langle \mathcal{D}c | \mathcal{D}\varphi \rangle_{\mathrm{L}^2(Q)} + \langle G(\varphi) | \lambda_1 \rangle_{\mathrm{L}^2(Q)} - \langle G(\varphi) | \lambda_2 \rangle_{\mathrm{L}^2(Q)} = \langle f | \mathcal{D}\varphi \rangle_{\mathrm{L}^2(Q)} \\ (\forall (q_1, q_2) \in \Lambda^2) & \begin{cases} \langle G(c) | q_1 - \lambda_1 \rangle_{\mathrm{L}^2(Q)} & \leq \langle \varepsilon_1 - b | q_1 - \lambda_1 \rangle_{\mathrm{L}^2(Q)} \\ -\langle G(c) | q_2 - \lambda_2 \rangle_{\mathrm{L}^2(Q)} & \leq \langle \varepsilon_2 - b | q_2 - \lambda_2 \rangle_{\mathrm{L}^2(Q)}. \end{cases} \end{cases} \tag{TCmf}$$

Lemma 4.1. *Assuming $b \in V_0(u,Q)$ and $a \in W^{1,\infty}(Q)$ are such that*

$$(\exists \alpha \in]0,+\infty[) \quad \alpha \leq a \quad \text{a.e.},$$

then the following inf − sup *inequality holds:*

$$(\exists \beta > 0) \quad \inf_{\psi \in L^2(Q), |\psi|_{L^2(Q)}=1} \quad \sup_{\varphi \in V_0(u,Q), |\varphi|_{1,\mathrm{div}u}=1} \langle G(\varphi)|\psi\rangle_{L^2(Q)} \geq \beta.$$

Proof. Given any such ψ, $|\psi|_{L^2(Q)} = 1$, define $Z = \mathrm{Ker}\, G \cap V_0(u,Q)$ and $Z^\perp$ to be the orthogonal of Z for $\langle \mathcal{D}\cdot|\mathcal{D}\cdot\rangle_{L^2(Q)}$. Set $\varphi \in Z^\perp$ such that $\mathcal{D}^*\mathcal{D}G(\varphi) = \psi$, then we get $\langle G(\varphi)|\psi\rangle_{L^2(Q)} = |G(\varphi)|^2_{1,\mathrm{div}u}$. Since $\mathcal{D}^*$ and G^{-1} are bounded we have

$$\begin{cases} |\psi|_{L^2(Q)} & \leq \quad \|\mathcal{D}^*\| \times |\mathcal{D}G(\varphi)|_{L^2(Q)} = \|\mathcal{D}^*\| \times |G(\varphi)|_{1,\mathrm{div}u} \\ |\varphi|_{1,\mathrm{div}u} & \leq \quad \|G^{-1}\| \times |G(\varphi)|_{1,\mathrm{div}u} \end{cases}$$

thus $\frac{1}{\|G^{-1}\|\|\mathcal{D}^*\|} \leq \frac{|G(\varphi)|_{1,\mathrm{div}u}}{|\varphi|_{1,\mathrm{div}u}}$ and the inf − sup inequality arises by rescaling. □

Theorem 4.2. (TCmf) *has a unique solution $(c,\lambda_1,\lambda_2) \in V_0(u,Q) \times L^2(Q)^2$. Moreover, this solution has the same c as the one given in Lemma 3.1.*

Proof. Using the inf − sup condition established in Lemma 4.1, the equivalence of the variational inequality with the mixed formulation for a one-sided constraint inequality is proved in [7]. It is straightforward to extend this result to the double-sided variational inequality (2). □

Remark 4.3. The constrained optimization approach for solving (TC) can readily be extended to the case of convex regular g functions. Unfortunately, the mixed formulation could not be applied in this case.

5 Numerical Approximation

We briefly explain here how a numerical approximation of the solution we propose can be readily derived. See, *e.g.*, [2] for the practical implementation of the efficient STILS scheme. Assume $\mathcal{T}_h$ is a conforming tetrahedral (for positivity) mesh of Q and define the following finite-dimensional spaces:

$$\begin{aligned} V_{0_h}(u,Q) &= \{v_h \in C^0(\overline{Q}) : (\forall K \in \mathcal{T}_h)\ v_{h|K} \in \mathrm{P}_1(\overline{K})\} \cap V_0(u,Q), \Lambda_h \\ &= \Lambda \cap V_{0_h}(u,Q), \end{aligned}$$

where $P_1(\overline{K})$ denotes the space of first-degree polynomials over $\overline{K}$. We then have the following property:

Proposition 5.1. *Assuming $b \in V_0(u,Q)$ and $a \in W^{1,\infty}(Q)$ are such that*

$$(\exists \alpha \in]0,+\infty[) \quad \alpha \leq a \quad \text{a.e.},$$

then the following inf – sup *inequality holds:*

$$(\exists \beta > 0) \qquad \inf_{\psi_h \in V_{0_h}(u,Q), |\psi_h|_{L^2(Q)}=1} \quad \sup_{\varphi_h \in V_{0_h}(u,Q), |\varphi_h|_{1,\mathrm{div}u}=1} \quad \langle G(\varphi_h)|\psi_h\rangle_{L^2(Q)} \geq \beta.$$

Proof. $|\cdot|_{1,\mathrm{div}u}$ is a norm and since there exists $c\left(\frac{1}{|a|_{W^{1,\infty}}}\right)$ such that

$$|w_h|_{1,\mathrm{div}u} \leq c\left(\frac{1}{|a|_{W^{1,\infty}}}\right)|G(w_h)|_{1,\mathrm{div}u} \tag{3}$$

and therefore the LAX-MILGRAM Lemma shows that, given any $\psi_h \in V_{0_h}(u,Q)\backslash\{0\}$,

$$(\exists! v_h \in V_{0_h}(u,Q))\ (\forall w_h \in V_{0_h}(u,Q)) \quad \langle \mathcal{D}(av_h)|\mathcal{D}(aw_h)\rangle_{L^2(Q)} = \langle aw_h|\psi_h\rangle_{L^2(Q)} \tag{4}$$

thus with $\psi_h = (\mathcal{D}G_h)^*\mathcal{D}G_h v_h$, we have $|\psi_h|_{L^2(Q)} \leq c_1|v_h|_{1,\mathrm{div}u}$ and, taking v_h as the test function in (4),

$$\frac{|v_h|^2_{1,\mathrm{div}u}}{c^2\left(\frac{1}{|a|_{W^{1,\infty}}}\right)} \leq |av_h|^2_{1,\mathrm{div}u} \leq \langle av_h|\psi_h\rangle_{L^2(Q)}$$

which establishes the discrete inf – sup condition. □

6 Conclusion

Let us end this note by taking advantage of Remark 3.3 in the case where K denotes the convex cone of non negative functions for proving that a time slabbing (see [2]) L^2 projection strategy is not a good strategy. Let $\rho \in K$ be a solution of

$$\begin{cases} t\partial_t\rho + \partial_x\rho &= x^2 - x \quad \text{in } Q = (0,1)\times(0,1) \\ c(0,t) &= 1/12 \quad \text{in } (0,1) \end{cases} \tag{TCDIV}$$

with the notation f: $(x,t) \mapsto (x^2 - x)$. We know from [5], that $\mathcal{D}^*$ is bijective. Thus, for $h \in L^2(Q)$ given, it is equivalent to find $c \in V_0(u,Q)$ satisfying:

$$(\forall \varphi \in V_0(u,Q)) \quad \langle \mathcal{D}c|\mathcal{D}\varphi\rangle_{L^2(Q)} = \langle h|\mathcal{D}\varphi\rangle_{L^2(Q)}$$

and to find $c \in V_0(u,Q)$ satisfying:

$$(\forall \varphi \in \mathrm{L}^2(Q)) \quad \langle \mathcal{D}c | \varphi \rangle_{\mathrm{L}^2(Q)} = \langle h | \varphi \rangle_{\mathrm{L}^2(Q)}.$$

From Remark 3.3 we deduce that the solution to the constrained optimization problem is to find $c \in V_0(u,Q)$ satisfying:

$$(\forall \varphi \in V_0(u,Q)) \langle \mathcal{D}c | \mathcal{D}\varphi \rangle_{\mathrm{L}^2(Q)} = \langle f^+ - \mathrm{sgn}^+(c) f^- | \mathcal{D}\varphi \rangle_{\mathrm{L}^2(Q)}. \tag{5}$$

The following iterative procedure can be applied for computing c, solution of (5).

Algorithm 6.1.

1. $n \leftarrow 0$; $c^n \leftarrow 1$;
2. compute $\tilde{c}$, solution of
$$(\forall \varphi \in V_0(u,Q)) \langle \mathcal{D}\tilde{c} | \mathcal{D}\varphi \rangle_{\mathrm{L}^2(Q)} = \langle f^+ - \mathrm{sgn}^+(\overline{c}^n) f^- | \mathcal{D}\varphi \rangle_{\mathrm{L}^2(Q)},$$
3. $n \leftarrow n+1$; $c^n \leftarrow \Pi_K(\tilde{c})$;
4. if $\|c^n - c^{n-1}\| \leq \varepsilon$ stop; else go to 2.

Indeed, this algorithm converges very quickly (after few iterations).

A STILS time slabbing L^2 projection strategy consists of splitting the domain $Q = \cup_{i=1,\dots,I}[0,1] \times [t_{i-1}, t_i]$. Problem (TCDIV) is solved successively in each slab $[0,1] \times [t_{i-1}, t_i]$ with a least squares formulation and then ρ_i is projected onto K. On the next slab, $\Pi_K(\rho_i)$ is taken as a boundary condition. In Figure 2 a two-slab L^2 projection strategy is depicted, and is compared with the solution obtained with Algorithm 6.1. Clearly, a partial L^2 projection strategy does not provide the solution of the variational inequality.

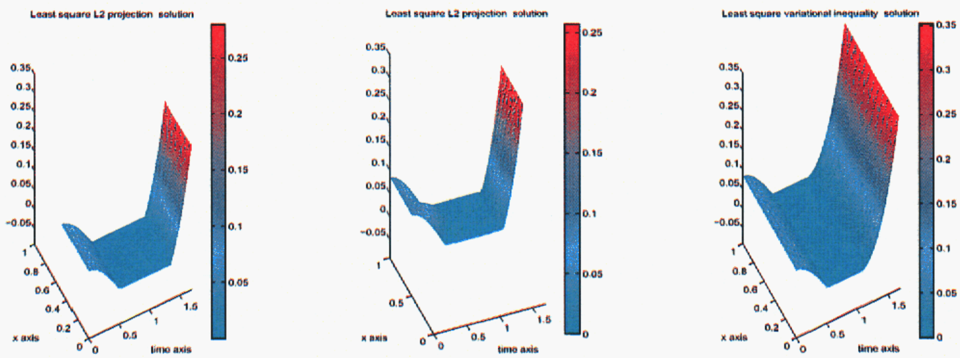

Figure 2. First L^2-projected slab solution (left), second L^2-projected slab solution (center), and STILS solution obtained with Algorithm 6.1 (right).

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