

A Dual-Mixed Hybrid Formulation for Fluid Mechanics Problems: Mathematical Analysis and Application to Semiconductor Process Technology

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Abstract

In this paper we propose a dual-mixed hybrid formulation capable of treating under a unified framework both compressible and incompressible problems in continuum mechanics. A theoretical analysis of the method is carried out and optimal error estimates are derived for both mixed and hybrid variables. The potentialities of the novel approach are exploited in the computation of the stress field required in the simulation of the thermal oxidation process in semiconductor technology. The numerical formulation is validated both on model problems in continuum mechanics and on a realistic example of the thermal oxidation process in a local oxidation structure (LOCOS).

Key words: Dual mixed-hybrid finite element methods; compressible and incompressible fluid-mechanical problems; thermal oxidation process; semiconductor technology.

1 Introduction and Motivation

In this paper we propose a dual mixed-hybrid (DMH) finite element formulation capable of dealing with both compressible and incompressible problems in continuum mechanics, providing at the same time an accurate representation of the stress field. The motivation underlying this research is to devise a flexible and reliable procedure for the simulation of physical systems involving materials with heterogeneous fluid-mechanical properties (for example, compressible and incompressible materials) using a unified numerical formulation.

This avoids in particular the escape of introducing quasi-incompressible approximations for handling the incompressible regime (such as the \bar{B} method, see [15], Sect.4.5.2, and [28], Sect.12.5.2) or the difficulty of adopting two separate computer codes, thus facing the problems arising from their proper coupling and maintenance. A significant example of the aforementioned situation occurs in the simulation of the thermal oxidation process in semiconductor device technology (see [20] and [22] for a more comprehensive mathematical presentation). In this industrial relevant application, the DMH formulation reveals to be an appropriate method to deal with the simultaneous presence of both compressible (silicon and silicon nitride) and incompressible (oxide) materials, providing at the same time an accurate approximation of the stress field which plays a primary role in the process evolution.

The DMH approach is based on the conservative form of the model continuum mechanics equations, and stems from a modified Hellinger-Reissner variational principle. The first modification consists in introducing a rotational parameter that weakly enforces the symmetry of the stress tensor [16]. At the discrete level, this has the effect of relieving from working with a discrete symmetric tensor function space. In this respect the DMH formulation may be regarded as a variant of the Plane Elasticity Element with Reduced Symmetry (PEERS) method [2,26]. It must be noticed that formulations based on the Hellinger-Reissner principles are not affected by locking phenomena in the quasi-incompressible and incompressible limit. An evidence of this statement can be found in the recent work [7], where an implementation of the PEERS method has been carried out, assessing the robustness of the method in the quasi-incompressible limit and deriving a-posteriori error estimates independent of the compressibility parameter. However, in the pure incompressible regime (Stokes problem), an additional constraint on the trace of the stress tensor must be enforced [4], which turns out turning into non-trivial difficulties at the discrete level. To overcome these difficulties, a second modification of the Hellinger-Reissner principle is carried out in the DMH formulation by introducing a pressure function to allow for a straightforward numerical treatment of the constraint of null volume variations [15]. In this latter case the pressure function has the physical meaning of hydrostatic pressure. Finally, a displacement interface variable (hybrid variable) is introduced to enforce the continuity of the normal stress across neighboring elements. This procedure is numerically equivalent to performing the hybridization of the corresponding dual-mixed formulation [1] and improves the computational efficiency of the method yielding a linear algebraic system in the interface displacements, pressure and rotation unknowns.

The paper is organized as follows: in Sect.2 we present the DMH formulation, proving existence and uniqueness of the solution of the continuous and discrete problems. In Sect.3 the error analysis of the method is carried out; in particular, we provide optimal error estimates for the approximation with a

superconvergence result for the hybrid variable. In Sect.4 we briefly describe the mathematical model of the thermal oxidation process and we discuss the algorithm implemented in the computer code to solve the fully coupled problem. In Sect.5 we present numerical results to validate the novel formulation, concerning first the sole fluid-mechanical formulation and then the simulation of a realistic thermal oxidation process. Finally, in Sect.6 we draw some conclusions and indicate some perspectives for the future work on this subject.

2 Dual mixed-hybrid formulation for the solution of the fluid-mechanical problem

The aim of this section is to present the DMH formulation for compressible and incompressible problems in continuum mechanics, stating existence and uniqueness results for both the associated continuous and discrete weak problems.

2.1 Functional setting and notation

Throughout the article Ω is an open bounded set in \mathbb{R}^2 with Lipschitz continuous boundary $\Gamma = \partial\Omega$, although the presentation of the method can be straightforwardly extended to the three-dimensional case. Let \mathcal{T}_h be a regular partition [9] of Ω into triangles K such that $\overline{\Omega} = \bigcup_{K \in \mathcal{T}_h} \overline{K}$ and let \mathcal{E}_h be the set of edges associated with \mathcal{T}_h . For each element $K \in \mathcal{T}_h$, we denote by ∂K the Lipschitz continuous boundary of K , by n_K the unit outward normal vector along the boundary ∂K and, for each $K, K' \in \mathcal{T}_h$ sharing an edge we set $e_{K-K'} = \partial K \cap \partial K'$. Moreover, if v is any function defined in Ω , we denote by v^K its restriction to the element K and by $v_{\partial K}$ its restriction on the element boundary ∂K .

Given an integer $m \geq 0$ and the real numbers $p, q \in [1, \infty)$, we define the following local space

$$W^{m,p}(K) = \{v \in L^p(K) \mid D^\alpha v \in L^p(K) \forall \alpha, |\alpha| \leq m\} \quad \forall K \in \mathcal{T}_h,$$

provided with the norm and seminorm

$$\|v\|_{m,p,K} = \left(\sum_{|\alpha| \leq m} \int_K |D^\alpha v|^p dx \right)^{1/p}, \quad |v|_{m,p,K} = \left(\sum_{|\alpha|=m} \int_K |D^\alpha v|^p dx \right)^{1/p}.$$

When $p = 2$, $W^{m,2}(K)$ is the usual $H^m(K)$ Sobolev space (see [18]) and the

simplified notation $\|\cdot\|_{m,K}$ and $|\cdot|_{m,K}$ will be used. We also introduce the local space

$$W_q(\operatorname{div}; K) = \left\{ \tau \in (L^q(K))^2 \mid \operatorname{div} \tau \in L^q(K) \right\},$$

provided with the norm

$$\|\tau\|_{q,\operatorname{div},K} = \left(\|\tau\|_{q,K}^q + \|\operatorname{div} \tau\|_{q,K}^q \right)^{1/q}.$$

When $q = 2$, the space $W_2(\operatorname{div}; K)$ is the Sobolev space $H(\operatorname{div}; K)$ (see [5]).

From now on, p and q will be chosen to be conjugate numbers, *i.e.*, $1/p + 1/q = 1$. It will be useful in the sequel to consider the space of the traces on ∂K of functions $v \in W^{1,p}(K)$ and $\tau \in W_q(\operatorname{div}; K)$. Notice that the trace $v|_{\partial K}$ belongs to the space $W^{1/q,p}(\partial K)$, while the normal trace $\tau n|_{\partial K}$ belongs to the space $W^{-1/q,q}(\partial K)$; the spaces $W^{1/q,p}(\partial K)$ and $W^{-1/q,q}(\partial K)$ are provided with the following norms

$$\|\tau n\|_{-1/q,q,\partial K} = \sup_{v \in W^{1,p}(K)} \frac{\langle \tau n, v \rangle_{\partial K}}{\|v\|_{1,p,K}}, \quad \forall \tau \in W_q(\operatorname{div}; K) \quad (1)$$

and

$$\|v\|_{1/q,p,\partial K} = \sup_{\tau \in W_q(\operatorname{div}; K)} \frac{\langle \tau n, v \rangle_{\partial K}}{\|\tau n\|_{-1/q,q,\partial K}}, \quad \forall v \in W^{1,p}(K). \quad (2)$$

Given the above functional setting, we can characterize the global space $W_q(\operatorname{div}; \Omega)$ as the space of the functions $\tau \in \prod_{K \in \mathcal{T}_h} W_q(\operatorname{div}; K)$ such that

$$\sum_{K \in \mathcal{T}_h} \langle \tau \cdot n, v \rangle_{\partial K} = 0 \quad \forall v \in W_0^{1,p}(\Omega), \quad (3)$$

where $W_0^{1,p}(\Omega)$ is the subspace of $W^{1,p}(\Omega)$ consisting of functions v such that $v = 0$ on Γ , and where $\langle \cdot, \cdot \rangle_{\partial K}$ denotes the duality pairing between $W^{-1/q,q}(\partial K)$ and $W^{1/q,p}(\partial K)$. Relation (3) extends to the space $W_q(\operatorname{div}; \Omega)$ the characterization of the space $H(\operatorname{div}; \Omega)$ which is essential in the construction of dual-hybrid methods (see [5], Ch.3, Prop.1.2.).

Proceeding as in [11,12], we assume henceforth that

$$4/3 < p < 2. \quad (4)$$

Under this condition, functions belonging to $W^{1/q,p}(\partial K)$ need not be continuous at the vertices of ∂K , unlike in standard dual-hybrid methods where the hybrid variable belongs to the space $W^{1/2,2}(\partial K) \equiv H^{1/2}(\partial K)$ and its approximation *must* be continuous at the vertices. This is the main reason for assuming the limitation (4), which allows instead for adopting *discontinuous piecewise finite elements* for the approximation of the hybrid variable on \mathcal{E}_h at the expense of a slightly stronger regularity on functions belonging

to $W_q(\text{div}; K)$ (indeed we have $q > 2$). While this latter extra-amount of regularity has no practical limiting consequences on the choice of the finite element spaces for the approximation of functions in $W_q(\text{div}; K)$, the relaxed continuity requirements for the hybrid variable has the advantage of producing an approximation of the normal stresses that is *continuous* on each edge of \mathcal{T}_h . This is not the case with standard hybrid methods, where this latter important conservation property is achieved only in an average sense over the patch of elements surrounding each node of the triangulation.

2.2 The continuum-mechanics problem in mixed form

Let us consider the linear elasticity problem in mixed form:

find (σ, u) such that

$$\begin{cases} \text{div } \sigma + f = 0 & \text{in } \Omega, \\ \sigma = 2\hat{\mu}\epsilon(u) + \hat{\lambda} \text{tr } \epsilon(u)\delta & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma, \end{cases} \quad (5)$$

where $\epsilon(u) = \frac{1}{2}(\nabla u + (\nabla u)^T)$ and $\hat{\lambda}$, $\hat{\mu}$ are the Lamè coefficients of the material. Homogeneous Dirichlet boundary conditions are assumed here only for ease of presentation; general mixed boundary conditions could be considered as well, as will be shown in the numerical experiments presented in Sect.5.

In order to derive the DMH formulation, we elaborate the constitutive equation (5)₂ as follows. We take the trace of (5)₂, yielding

$$\text{tr } \epsilon(u) = \frac{\text{tr } \sigma}{2(\hat{\lambda} + \hat{\mu})} \quad (6)$$

and we introduce the *pressure parameter*

$$p = -\frac{1}{2}\text{tr } \sigma. \quad (7)$$

Substituting these quantities back in (5)₂, we obtain the following expression for the constitutive law

$$\sigma = 2\hat{\mu}\epsilon(u) - \frac{\hat{\lambda}}{(\hat{\lambda} + \hat{\mu})}p\delta.$$

System (5) can thus be rewritten as

$$\begin{cases} \operatorname{div} \sigma + f = 0 & \text{in } \Omega, \\ \sigma = 2\widehat{\mu}\epsilon(u) - \frac{\widehat{\lambda}}{(\widehat{\lambda} + \widehat{\mu})}p\delta & \text{in } \Omega, \\ p = -\frac{1}{2}\operatorname{tr} \sigma & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma. \end{cases} \quad (8)$$

System (8) is the starting point for introducing the DMH formulation. It is easy to verify that for $\widehat{\lambda} \rightarrow +\infty$ system (8) can be conveniently interpreted as the conservative form of the Stokes equations in fluid dynamics

$$\begin{cases} \operatorname{div} (-2\nu\epsilon(u) + p\delta) = f & \text{in } \Omega, \\ \operatorname{div} u = 0 & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma, \end{cases} \quad (9)$$

where $\nu = \widehat{\mu}$ is the kinematic viscosity and u is to be intended as a velocity field. Indeed, from (6) and (7) we have

$$\operatorname{tr} \epsilon(u) = \operatorname{div} u = -\frac{p}{\widehat{\lambda} + \widehat{\mu}},$$

that for $\widehat{\lambda} \rightarrow +\infty$ recovers the incompressibility constraint $\operatorname{div} u = 0$. Notice that only in this latter case the pressure parameter p assumes the meaning of hydrostatic pressure (see also [15]).

2.3 Formulation of the problem with Lagrangian multipliers

We define the following function spaces

$$\begin{aligned} \Sigma &= \prod_{K \in \mathcal{T}_h} (W_q(\operatorname{div}; K))^2, & V &= (L^q(\Omega))^2, \\ \Lambda &= \left\{ \mu \in \prod_{K \in \mathcal{T}_h} (W^{1/q,p}(\partial K))^2, \mu^K = \mu^{K'} \text{ on } e_{K-K'}, \forall K, K' \in \mathcal{T}_h, \right. \\ &\quad \left. \mu^K = 0 \text{ on } \partial K \cap \Gamma, \forall K \in \mathcal{T}_h \right\}, \\ W &= L^q(\Omega), & Q &= L^q(\Omega) \cap L_0^2(\Omega), & \widehat{M} &= V \times \Lambda \times W, & M &= \widehat{M} \times Q, \end{aligned} \quad (10)$$

where $L_0^2(\Omega)$ is the subspace of $L^2(\Omega)$ of functions with zero mean value over Ω . Next, we let $\tilde{\tau} \equiv \tau \in \Sigma$, $\tilde{v} = (v, \mu, \theta) \in \tilde{M}$, $\tilde{v} = (\hat{v}, q) \in M$ and we introduce the following continuous bilinear forms $a(\cdot, \cdot)$, $b(\cdot, \cdot)$ and $c(\cdot, \cdot)$ defined respectively on $\Sigma \times \Sigma$, $\Sigma \times M$ and $M \times M$:

$$\left\{ \begin{array}{l} a(\tilde{\sigma}, \tilde{\tau}) = \frac{1}{2\hat{\mu}} \int_{\Omega} \sigma : \tau \, dx, \quad b(\tilde{v}, \tilde{\tau}) = b_1(\tilde{v}, \tilde{\tau}) + b_2(\tilde{v}, \tilde{\tau}), \\ b_1(\tilde{v}, \tilde{\tau}) = \sum_{K \in \mathcal{T}_h} \int_K v \cdot \operatorname{div} \tau \, dx - \sum_{K \in \mathcal{T}_h} \int_{\partial K} \mu \cdot (\tau n) \, ds + \int_{\Omega} \theta \operatorname{as} \tau \, dx, \\ b_2(\tilde{v}, \tilde{\tau}) = \int_{\Omega} \frac{\rho_{\hat{\lambda}}}{2} q \operatorname{tr} \tau \, dx, \\ c(\tilde{u}, \tilde{v}) = \int_{\Omega} \rho_{\hat{\lambda}} p q \, dx, \end{array} \right. \quad (11)$$

where $\sigma : \tau = \sum_{i,j=1}^2 \sigma_{ij} \tau_{ij}$, $\operatorname{as} \tau = \tau_{21} - \tau_{12}$ and $\rho_{\hat{\lambda}} = \hat{\lambda} / (\hat{\mu}(\hat{\lambda} + \hat{\mu}))$ (in the incompressible case we have $\rho_{\infty} = 1/\hat{\mu}$).

The DMH formulation of problem (5) reads:

find $(\tilde{\sigma} \equiv \sigma, \tilde{u} = (u, \lambda, \omega, p)) \in (\Sigma \times M)$, such that

$$\left\{ \begin{array}{l} a(\tilde{\sigma}, \tilde{\tau}) + b(\tilde{u}, \tilde{\tau}) = 0 \quad \forall \tilde{\tau} \in \Sigma, \\ b(\tilde{\sigma}, \tilde{v}) + c(\tilde{u}, \tilde{v}) = \mathcal{F}(\tilde{v}) \quad \forall \tilde{v} \in M, \end{array} \right. \quad (12)$$

where $\mathcal{F}(\tilde{v}) = - \int_{\Omega} f \cdot v \, dx$ and $f \in (L^p(\Omega))^2$.

Some comments on the meaning of the variables in (12) are in order.

The variable p is a pressure function that in the incompressible limit ($\hat{\lambda} = +\infty$) represents the hydrostatic pressure. In this latter case an undetermination on $\int_{\Omega} \operatorname{tr} \sigma \, dx$, *i.e.* on the mean value of p , arises. The undetermination can be solved by imposing *a-priori* the side condition $p \in L_0^2(\Omega)$. This latter procedure allows in turn for a straightforward numerical treatment of the constraint of null volume variations, that is easier to deal with than the corresponding condition on the trace of the stress tensor σ [2]. If $\hat{\lambda} < +\infty$, since $p = -\frac{1}{2} \operatorname{tr} \sigma =$ a.e. in Ω , taking $\tau = \delta$ in (12)₁ yields $\operatorname{tr} \sigma \in L_0^2(\Omega)$ and thus $p \in L_0^2(\Omega)$. This is the reason why p is sought in the space $L^q(\Omega) \cap L_0^2(\Omega)$ for every value of the compressibility parameter $\hat{\lambda}$, even when it is redundant (see [4] for a similar discussion of this subject).

The variable ω is a rotational parameter that avoids requesting the stress tensor to be sought *a priori* in a symmetric function space.

Finally, the hybrid variable λ is the Lagrangian multiplier that enforces back

the continuity of the normal component of the stress tensor across the interelement interfaces.

2.4 Existence and uniqueness of the solution of the DMH formulation

It is not hard to see that if (u^*, σ^*) is the solution of problem (5) such that $\sigma^* \in (W_q(\text{div}; \Omega))^2$ and such that $\text{tr } \sigma^* \in (L^q(\Omega) \cap L_0^2(\Omega))$, then $(\tilde{\sigma} = \sigma^*; \tilde{u} = (u^*, u_{\partial K}^*, \frac{1}{2}\text{curl } u^*, p = -\frac{1}{2}\text{tr } \sigma^*))$ is a solution of (12), where $\forall \phi = (\phi_1, \phi_2) \in (H^1(\Omega))^2$ we have $\text{curl } \phi = (\frac{\partial \phi_2}{\partial x_1} - \frac{\partial \phi_1}{\partial x_2})$.

To assess the uniqueness of the solution of problem (12), we set $f = 0$, take $\tilde{\tau} = \tilde{\sigma}$ in $(12)_1$, $\tilde{v} = \tilde{u}$ in $(12)_2$ and subtract $(12)_2$ from $(12)_1$, yielding

$$a(\sigma, \sigma) - c(p, p) = 0. \quad (13)$$

We can rewrite (13) as

$$\tilde{a}(\sigma, \sigma) = 0, \quad (14)$$

where

$$\tilde{a}(\tau, \tau) = \frac{1}{2\hat{\mu}} \|\tau^D\|_{0,\Omega}^2 + \frac{1}{4(\hat{\lambda} + \hat{\mu})} \|\text{tr } \tau\|_{0,\Omega}^2 \quad \forall \tau \in \Sigma,$$

having defined for every $\tau \in \Sigma$ the deviatoric part of τ as $\tau^D = \tau - \frac{1}{2} \text{tr } (\tau) \delta$.

In the compressible regime ($\hat{\lambda} < +\infty$), equation (14) immediately yields $\sigma = 0$ and consequently $p = 0$. In the incompressible regime ($\hat{\lambda} = +\infty$), equation (14) provides a control only for the deviatoric part of σ . To ensure control on the complete tensor, we recall that, since $\text{div } \sigma = 0$ in Ω ($f = 0$) and $\text{tr } \sigma \in L_0^2(\Omega)$, there exists a positive constant C such that (see [3])

$$\|\sigma\|_{0,\Omega} \leq C \|\sigma^D\|_{0,\Omega}$$

(see [5] Prop. 3.1 p.161). This allows us to conclude that $\sigma = 0$ also in the incompressible case. From this latter result, it immediately follows that $p = 0$ as well.

In order to show that also $u = 0$, $\lambda = 0$ and $\omega = 0$, we must check the inf-sup condition for the bilinear form $b_1(\cdot, \cdot)$. To do this, we use the following proposition (see [12] for a proof):

Proposition 1 *There exists a positive constant C such that*

$$\sup_{\tilde{\tau} \in \Sigma, \tilde{\tau} \neq 0} \frac{b_1(\hat{v}, \tilde{\tau})}{\|\tilde{\tau}\|_{0,\Omega}} \geq C(\|v\|_{0,\Omega} + \|\theta\|_{0,\Omega}) \quad \forall \hat{v} \in \widehat{M}.$$

We are now in a position to state the following existence and uniqueness result:

Theorem 2.1 *Suppose that the solution (u, σ) of problem (5) has the regularity*

$$\sigma \in (W_q(\operatorname{div}; \Omega))^2, \quad \operatorname{tr} \sigma \in L^q(\Omega) \cap L_0^2(\Omega).$$

Then $(\tilde{\sigma} = \sigma; \tilde{u} = (u, u_{\partial K}, \frac{1}{2} \operatorname{curl} u, -\frac{1}{2} \operatorname{tr} \sigma))$ is the unique solution of problem (12).

2.5 Finite element discretization of the DMH formulation

This section concerns with the numerical approximation of problem (12). For $k \geq 0$, we denote by $\mathbb{P}_k(K)$ the space of polynomials in two variables of total degree at most k on the element K and by $R_k(\partial K)$ the space of polynomials of total degree at most k on each edge of K . Notice that functions belonging to $R_k(\partial K)$ need not to be continuous at the vertices of ∂K . Furthermore, we denote by $\mathbb{D}(K) = (\mathbb{RT}_0(K) \oplus \mathcal{B}_K)^2$, where $\mathbb{RT}_0(K)$ is the lowest order Raviart-Thomas finite element space [23] on K and $\mathcal{B}_K = \operatorname{curl}(b_K)$, b_K being the cubic bubble function on K . The finite element spaces for the DMH approximation are defined as follows:

$$\begin{aligned} \Sigma_h &= \left\{ \tau \in \Sigma \mid \tau^K \in \mathbb{D}(K) \forall K \in \mathcal{T}_h \right\}, \quad V_h = \left\{ v \in V \mid v^K \in (\mathbb{P}_0(K))^2 \forall K \in \mathcal{T}_h \right\}, \\ \Lambda_h &= \left\{ \mu \in \Lambda \mid \mu_{\partial K} \in (R_0(\partial K))^2 \forall K \in \mathcal{T}_h \right\}, \quad W_h = \left\{ \theta \in C^0(\bar{\Omega}) \mid \theta^K \in \mathbb{P}_1(K) \forall K \in \mathcal{T}_h \right\}, \\ Q_h &= \left\{ q \in Q \mid q^K \in \mathbb{P}_0(K) \quad \forall K \in \mathcal{T}_h \right\}, \\ \widehat{M}_h &= V_h \times \Lambda_h \times W_h, \quad \widehat{M}_h = M_h \times Q_h. \end{aligned} \tag{15}$$

The finite element spaces Σ_h, V_h, Λ_h and W_h are the same as in [2] except for the space Q_h , since the pressure variable is not introduced in that formulation. The pressure variable is instead introduced in [11,12] in a similar formulation but considering a different constitutive law for the stress σ , that in these references is defined as $\sigma = 2\widehat{\mu}\epsilon(u)$. This latter choice implies that σ does not account for volumetric variations, that are instead represented by the pressure, but only for deviatoric stresses. However, in the definition of the complete stress tensor *both* contributions must appear, this reflecting into a rather involved functional and discrete representation of the spaces Σ and Σ_h (see [12], definition 2.1 and Example 3.1). On the other hand, in the DMH formulation, which is more akin to the PEERS method, the introduction of the pressure variable is carried out according to a straightforward physical definition which extends to the dual-mixed formulation of the elasticity problem the original approach proposed by Herrmann in [17] in the context of displacement-based formulations.

A final remark is in order concerning with the rotation finite element space W_h that consists of *nodally continuous functions* over $\bar{\Omega}$. We give here the following physical interpretation of this statement. As a matter of fact, the simplest choice

$$W_h = \{\theta \in W \mid \theta|_K \in \mathbb{P}_0(K) \forall K \in \mathcal{T}_h\}$$

leads to undesired *rigid body motions* (mechanisms) of rotational type (see Fig.1). This suggests that some kind of rotational continuity between neighboring triangles must be enforced, as is the case of the space W_h used in the present formulation.

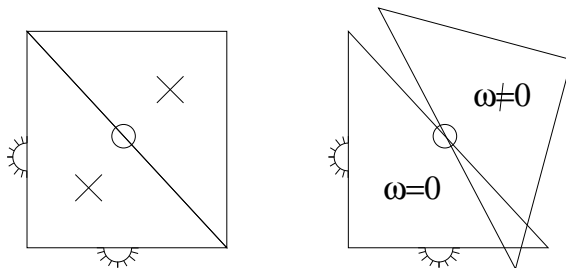


Figure 1. Discontinuous approximate rotations lead to the appearance of rigid body motions. In the schematic representation, the hinges denote the variable λ_h , while crosses denote the variable ω_h .

Having introduced the finite element spaces (15), problem (12) is discretized by the following one:

find $(\tilde{\sigma}_h \equiv \sigma_h, \tilde{u}_h = (u_h, \lambda_h, \omega_h, p_h)) \in (\Sigma_h \times M_h)$, such that

$$\begin{cases} a(\tilde{\sigma}_h, \tilde{\tau}_h) + b(\tilde{u}_h, \tilde{\tau}_h) = 0 & \forall \tilde{\tau}_h \in \Sigma_h, \\ b(\tilde{\sigma}_h, \tilde{v}_h) + c(\tilde{u}_h, \tilde{v}_h) = \mathcal{F}(\tilde{v}_h) & \forall \tilde{v}_h \in M_h. \end{cases} \quad (16)$$

The proof of the uniqueness of the solution of problem (16) follows the same lines as in the continuous case. Setting $f = 0$ in (16), we first check that

$$a(\sigma_h, \sigma_h) - c(p_h, p_h) = 0 \quad \text{implies} \quad \sigma_h = 0, p_h = 0. \quad (17)$$

To do this, it is useful to recall that the space $L_0^2(\Omega)$ is isomorphically equivalent to the space $L^2(\Omega)/\mathbb{R}$. At the discrete level, working in the space

$$Q_h = \left\{ q \in (L^q(\Omega) \cap L^2(\Omega)/\mathbb{R}) \mid q^K \in \mathbb{P}_0(K) \forall K \in \mathcal{T}_h \right\}$$

is equivalent to prescribing the value $p_h = p^*$ on a certain element K^* of the triangulation, p^* being an arbitrary constant (see for example [19], Sect.9.3).

Without loss of generality, we can set $p^* = 0$. Then, we can take in equation (16)₂ $\tilde{v}_h = (0, 0, 0, 1_K)$, with $1_K = 1$ on K , $K \neq K^*$ and 0 elsewhere, obtaining

$$p_h^K = -\frac{1}{2|K|} \int_K \operatorname{tr} \sigma_h dx \quad \forall K \in \mathcal{T}_h, K \neq K^*.$$

Substituting this latter relation back in (17), we get

$$\begin{aligned} 0 &= \sum_{K \in \mathcal{T}_h} \int_K \frac{1}{2\hat{\mu}} \sigma_h : \sigma_h dx - \sum_{K \in \mathcal{T}_h, K \neq K^*} \int_K \frac{\rho_{\hat{\lambda}}}{4|K|^2} \left(\int_K \operatorname{tr} \sigma_h dx \right)^2 dx \\ &\geq \sum_{K \in \mathcal{T}_h} \left(\int_K \frac{1}{2\hat{\mu}} \sigma_h : \sigma_h dx - \int_K \frac{\rho_{\hat{\lambda}}}{4|K|^2} \left(\int_K \operatorname{tr} \sigma_h dx \right)^2 dx \right) \\ &\geq \sum_{K \in \mathcal{T}_h} \left(\int_K \frac{1}{2\hat{\mu}} \sigma_h : \sigma_h dx - \int_K \frac{\rho_{\hat{\lambda}}}{4|K|} \int_K (\operatorname{tr} \sigma_h)^2 dx \right) \\ &= \sum_{K \in \mathcal{T}_h} \left(\int_K \frac{1}{2\hat{\mu}} \sigma_h^D : \sigma_h^D dx - \int_K \frac{1}{4(\hat{\lambda} + \hat{\mu})} (\operatorname{tr} \sigma_h)^2 dx \right) = \tilde{a}(\sigma_h, \sigma_h), \end{aligned}$$

where we have used the fact that

$$\left(\int_K \operatorname{tr} \sigma_h dx \right)^2 \leq |K| \int_K (\operatorname{tr} \sigma_h)^2 dx \quad (18)$$

From the above inequality and from the definition of $\tilde{a}(\cdot, \cdot)$, it immediately follows that $\sigma_h = 0$ and $p_h = 0$, irrespectively of the value of the compressibility parameter $\hat{\lambda}$.

In order to show that also $u_h = 0$, $\lambda_h = 0$ and $\omega_h = 0$, we must check the discrete inf-sup condition for the bilinear form $b_1(\cdot, \cdot)$. For this we use the following proposition (see [12] for a proof):

Proposition 2 *There exists a positive constant C such that*

$$\sup_{\tilde{\tau}_h \in \Sigma_h, \tilde{\tau}_h \neq 0} \frac{b_1(\hat{v}, \tilde{\tau}_h)}{\|\tilde{\tau}_h\|_{0,\Omega}} \geq C(\|v_h\|_{0,\Omega} + \|\theta_h\|_{0,\Omega}) \quad \forall \hat{v}_h \in \widehat{M}_h.$$

We are now in a position to state the existence and uniqueness result:

Theorem 2.2 *There exists a unique element $(\tilde{\sigma}_h, \tilde{u}_h) \in (\Sigma_h \times M_h)$ satisfying (16).*

3 Error analysis

The subsequent analysis is divided into several steps. First, we introduce suitable projection and interpolation operators. Then we obtain optimal error estimates for σ, p, u and ω . Finally, we derive optimal error estimates for the L^2 projection of u and for the hybrid variable λ .

3.1 Projection and interpolation operators

In order to carry out the error analysis for the DMH formulation, we need to introduce appropriate projection and interpolation operators. First, we define the linear operator $\Pi_K^1 : W_q(\text{div}; K)^2 \rightarrow \Sigma_h(K)$ satisfying the orthogonality relation

$$\int_{\partial K} (\Pi_K^1 \tau - \tau) n \cdot r_0 = 0 \quad \forall r_0 \in (R_0(\partial K))^2, \quad \forall K \in \mathcal{T}_h \quad (19)$$

and satisfying for all $\tau \in (H^1(K))^4$, $\text{div} \tau \in (H^1(K))^2$ the approximation properties (see [25], Chapt.6, Theorem 6.3)

$$\begin{aligned} \|\tau - \Pi_K^1 \tau\|_{0,K} &\leq Ch_K |\tau|_{1,K}, \\ \|\text{div}(\tau - \Pi_K^1 \tau)\|_{0,K} &\leq Ch_K^l |\text{div} \tau|_{1,K}, \quad l = 0, 1, \end{aligned} \quad (20)$$

where C is a constant independent of K and h_K is the diameter of K . From the operator Π_K^1 , for all $\tau \in W_q(\text{div}; K)^2 \cap (L^q(\Omega))^4$, we construct the global operator Π_h^1 as

$$\Pi_h^1 \tau|_K = \Pi_K^1 \tau \quad \forall K \in \mathcal{T}_h.$$

Moreover, we denote by P_h^0 the projection operator from $(L^2(\Omega))^2$ onto V_h such that, for all $v \in (L^2(\Omega))^2$, we have

$$\int_K (P_h^0 v - v) \cdot p_0 \, dx = 0 \quad \forall p_0 \in (\mathbb{P}_0(K))^2, \quad \forall K \in \mathcal{T}_h,$$

and by ρ_h^0 the projection operator from $\prod_{K \in \mathcal{T}_h} (L^2(\partial K))^2$ onto Λ_h such that, for all $\mu \in \prod_{K \in \mathcal{T}_h} (L^2(\partial K))^2$, we have

$$\int_{\partial K} (\rho_h^0 \mu - \mu) \cdot r_0 \, dx = 0 \quad \forall r_0 \in (R_0(\partial K))^2, \quad \forall K \in \mathcal{T}_h.$$

Then, for all $q \in L^2(\Omega)$, we introduce the following projection operator from $L^2(\Omega)$ onto Q_h

$$s_h q = \rho_h q - \frac{1}{|\Omega|} \int_{\Omega} \rho_h q \, dx,$$

where $|\Omega| = \text{meas}(\Omega)$ and ρ_h is the L^2 projection from $\prod_{K \in \mathcal{T}_h} L^2(K)$ onto $\prod_{K \in \mathcal{T}_h} \mathbb{P}_0(K)$. Finally, we let $\rho_h^{1,c}$ be the Clément interpolation operator (see [9], Sect.17) from $H^1(\Omega)$ onto W_h such that, for all $\eta \in H^1(\Omega)$, we have

$$|\eta - \rho_h^{1,c}\eta|_{m,\Omega} \leq Ch^{1-m}|\eta|_{1,\Omega}, \quad m = 0, 1.$$

3.2 Error estimates

We start with the following result.

Lemma 3.1 *If the triangulation \mathcal{T}_h is regular, then there exists an operator $\Pi_h : \Sigma \rightarrow \Sigma_h$ such that, for all $\tilde{\tau} \equiv \tau \in \Sigma$, we have*

$$b_1(\tilde{\tau} - \Pi_h \tilde{\tau}, \tilde{v}_h) = 0 \quad \forall \tilde{v}_h \in M_h. \quad (21)$$

Moreover, if $\tilde{\tau} \in (H^1(\Omega))^4$, we have

$$\|\tilde{\tau} - \Pi_h \tilde{\tau}\|_{0,\Omega} \leq Ch|\tau|_{1,\Omega}, \quad (22)$$

where C is a constant independent of h .

Proof. Following [12], we let s be the mean value of $\text{as}(\tau - \Pi_h^1 \tau)$ on Ω and $\beta = \text{as}(\tau - \Pi_h^1 \tau) - s$. Thus, there exists $w \in (H_0^1(\Omega))^2$ such that $\text{div } w = \beta$ and $\|w\|_{1,\Omega} \leq C\|\beta\|_{0,\Omega}$ (see [14], Lemma 2.2 and Corollary 2.4), from which it follows that $\|w\|_{1,\Omega} \leq C\|\tau - \Pi_h^1 \tau\|_{0,\Omega}$. We now exploit the correspondence between the finite element spaces used in the present work for the stress and the rotation fields and the finite element spaces used in the *MINI* element [5] to approximate the velocity and the pressure fields in the Stokes problem. The stability of the *MINI* discretization allows us to conclude that the approximate velocity $w_h = (w_h^1, w_h^2)$, with

$$w_h \in \left\{ z \in (C^0(\bar{\Omega}))^2, z^K \in (\mathbb{P}_1(K) \oplus \mathcal{B})^2, \forall K \in \mathcal{T}_h \right\}$$

is such that $\int_{\Omega} \text{div}(w - w_h)\xi_h dx = 0$ for all piecewise linear continuous functions ξ_h and $\|w_h\|_{1,\Omega} \leq C\|w\|_{1,\Omega}$. Choosing

$$\Pi_h \tilde{\tau} = \Pi_h^1 \tilde{\tau} + (\text{curl } w_h^1, \text{curl } w_h^2) + (s/2)\chi,$$

it is immediate to check that (21) is satisfied. Observing now that $\|\tilde{\tau} - \Pi_h \tilde{\tau}\|_{0,\Omega} \leq C\|\tilde{\tau} - \Pi_h^1 \tilde{\tau}\|_{0,\Omega}$ and using property (20)₁, we eventually end up with (22). \square

We are now in a position to prove the following result.

Theorem 3.1 *Let $(\tilde{\sigma}, \tilde{u})$ be the solution of problem (12) and $(\tilde{\sigma}_h, \tilde{u}_h)$ be the solution of problem (16). If $\sigma \in (H^1(\Omega))^4$, $p \in (H^1(\Omega) \cap L_0^2(\Omega))$ and $\omega \in$*

$H^1(\Omega)$, then there exists a constant C independent of h such that

$$\|\sigma - \sigma_h\|_{0,\Omega} + \|p - p_h\|_{0,\Omega} \leq Ch(|\sigma|_{1,\Omega} + |p|_{1,\Omega} + |\omega|_{1,\Omega}), \quad (23)$$

$$\|u - u_h\|_{0,\Omega} \leq Ch(|\sigma|_{1,\Omega} + |p|_{1,\Omega} + |u|_{1,\Omega} + |\omega|_{1,\Omega}), \quad (24)$$

$$\|\omega - \omega_h\|_{0,\Omega} \leq Ch(|\sigma|_{1,\Omega} + |p|_{1,\Omega} + |\omega|_{1,\Omega}). \quad (25)$$

Proof. From (12) and (16) we obtain the error equations

$$\begin{cases} b(\tilde{\sigma} - \tilde{\sigma}_h, \tilde{v}_h) = -c(\tilde{u} - \tilde{u}_h, \tilde{v}_h) & \forall \tilde{v}_h \in V_h, \\ a(\tilde{\sigma} - \tilde{\sigma}_h, \tilde{\tau}_h) + b(\tilde{u} - \tilde{u}_h, \tilde{\tau}_h) = 0 & \forall \tilde{\tau}_h \in \Sigma_h. \end{cases} \quad (26)$$

Denote by $P_h \tilde{u} = (P_h^0 u, \rho_h^0 \lambda, \rho_h^{1,c} \omega, s_h p)$ the projection of \tilde{u} onto the space M_h . It is immediate to check that $P_h \tilde{u}$ satisfies

$$b(\tilde{\tau}_h, P_h \tilde{u} - \tilde{u}) = \int_{\Omega} \frac{\rho_{\hat{\lambda}}}{2} (p - s_h p) \operatorname{tr}(\tilde{\tau}_h) dx + \int_{\Omega} (\omega - \rho_h^{1,c} \omega) \operatorname{as}(\tilde{\tau}_h) dx, \quad \forall \tilde{\tau}_h \in \Sigma_h. \quad (27)$$

Using (21) and taking $\tau_h = \Pi_h \tilde{\sigma} - \tilde{\sigma}_h$ we get

$$\begin{cases} b(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h, \tilde{v}_h) = \int_{\Omega} \frac{\rho_{\hat{\lambda}}}{2} q_h \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}) dx - c(\tilde{u} - \tilde{u}_h, \tilde{v}_h) & \forall \tilde{v}_h \in M_h, \\ a(\tilde{\sigma} - \tilde{\sigma}_h, \Pi_h \tilde{\sigma} - \tilde{\sigma}_h) + b(P_h \tilde{u} - \tilde{u}_h, \Pi_h \tilde{\sigma} - \tilde{\sigma}_h) = b(P_h \tilde{u} - \tilde{u}, \Pi_h \tilde{\sigma} - \tilde{\sigma}_h), \end{cases} \quad (28)$$

yielding for (28)₂

$$\begin{aligned} a(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h, \Pi_h \tilde{\sigma} - \tilde{\sigma}_h) &= a(\Pi_h \tilde{\sigma} - \tilde{\sigma}, \Pi_h \tilde{\sigma} - \tilde{\sigma}_h) \\ &- \left(\int_{\Omega} \frac{\rho_{\hat{\lambda}}}{2} (p - s_h p) \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx + \int_{\Omega} (\omega - \rho_h^{1,c} \omega) \operatorname{as}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx \right) \\ &+ \int_{\Omega} \frac{\rho_{\hat{\lambda}}}{2} (s_h p - p_h) \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}) dx - \int_{\Omega} \rho_{\hat{\lambda}} (p - p_h) (s_h p - p_h) dx. \end{aligned} \quad (29)$$

To proceed, we need to establish an estimate for the error on the pressure variable. Setting $\tilde{v}_h = (0, 0, 0, q_h)$ in (26)₁ yields the following error equation for the pressure constitutive relation

$$\int_{\Omega} \rho_{\hat{\lambda}} \left[(p - p_h) + \frac{1}{2} \operatorname{tr}(\sigma - \sigma_h) \right] q_h dx = 0 \quad \forall q_h \in Q_h. \quad (30)$$

Taking $q_h = s_h p - p_h$ in (30) and performing some manipulations we get

$$\rho_{\hat{\lambda}} \int_{\Omega} (s_h p - p_h) \left[\frac{1}{2} \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}) - (p - p_h) \right] dx = \rho_{\hat{\lambda}} \int_{\Omega} (s_h p - p_h) \frac{1}{2} \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx.$$

The above relation allows to conveniently reformulate (29) as

$$\begin{aligned}
& a(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h, \Pi_h \tilde{\sigma} - \tilde{\sigma}_h) + \int_{\Omega} \frac{\rho_{\hat{\lambda}}}{2} (s_h p - p_h) \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx \\
&= a(\Pi_h \tilde{\sigma} - \tilde{\sigma}, \Pi_h \tilde{\sigma} - \tilde{\sigma}_h) + \int_{\Omega} \frac{\rho_{\hat{\lambda}}}{2} (s_h p - p) \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx \quad (31) \\
&+ \int_{\Omega} (\rho_h^{1,c} \omega - \omega) \operatorname{as}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx.
\end{aligned}$$

Let us now obtain a relation between $s_h p - p_h$ and $\operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h)$ over each element $K \in \mathcal{T}_h, K \neq K^*$. Taking $q_h = 1^K, K \neq K^*$, after some algebra relation (30) gives $\forall K \in \mathcal{T}_h, K \neq K^*$

$$(s_h p - p_h)|_K = -\frac{1}{2|K|} \int_K \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx + \frac{1}{|K|} \left(\int_K (s_h p - p) dx + \int_K \frac{1}{2} \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}) dx \right).$$

This latter relation can be used in the second integral at the left hand side of (31), to obtain

$$\begin{aligned}
& \int_{\Omega} \frac{\rho_{\hat{\lambda}}}{2} (s_h p - p_h) \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx = \sum_{K \neq K^*} \frac{\rho_{\hat{\lambda}}}{2} (s_h p - p_h)|_K \int_K \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx \\
&= \sum_{K \neq K^*} \left[-\frac{\rho_{\hat{\lambda}}}{4|K|} \left(\int_K \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx \right)^2 \right. \\
&\left. + \frac{\rho_{\lambda}}{2|K|} \left(\int_K (s_h p - p) dx + \int_K \frac{1}{2} \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}) dx \right) \int_K \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx \right],
\end{aligned}$$

that yields the following form of (31)

$$\begin{aligned}
& \int_{\Omega} \frac{1}{2\hat{\mu}} (\Pi_h \tilde{\sigma} - \tilde{\sigma}_h)^2 dx - \sum_{K \neq K^*} \frac{\rho_{\hat{\lambda}}}{4|K|} \left(\int_K \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx \right)^2 \\
&= a(\Pi_h \tilde{\sigma} - \tilde{\sigma}, \Pi_h \tilde{\sigma} - \tilde{\sigma}_h) - \sum_{K \in \mathcal{T}_h, K \neq K^*} \frac{\rho_{\hat{\lambda}}}{2|K|} \left(\int_K (s_h p - p) dx \right. \\
&\left. + \int_K \frac{1}{2} \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}) dx \right) \int_K \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx \quad (32) \\
&+ \int_{\Omega} \frac{\rho_{\hat{\lambda}}}{2} (s_h p - p) \operatorname{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx + \int_{\Omega} (\rho_h^{1,c} \omega - \omega) \operatorname{as}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx \Big].
\end{aligned}$$

Using again (18) and Lemma 4.3 of [2], we obtain the following coerciveness result for the left hand side of (32)

$$\begin{aligned}
& \int_{\Omega} \frac{1}{2\hat{\mu}} (\Pi_h \tilde{\sigma} - \tilde{\sigma}_h)^2 dx - \sum_{K \neq K^*} \frac{\rho_{\hat{\lambda}}}{4|K|} \left(\int_K \text{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h) dx \right)^2 \\
& \geq \int_{\Omega} \frac{1}{2\hat{\mu}} (\Pi_h \tilde{\sigma} - \tilde{\sigma}_h)^2 dx - \frac{\rho_{\hat{\lambda}}}{4} \int_{\Omega} (\text{tr}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h))^2 dx \\
& \equiv \tilde{a}(\Pi_h \tilde{\sigma} - \tilde{\sigma}_h, \Pi_h \tilde{\sigma} - \tilde{\sigma}_h) \geq C_{\hat{\mu}}(\Omega) \|\Pi_h \tilde{\sigma} - \tilde{\sigma}_h\|_{0,\Omega}^2,
\end{aligned}$$

where $C_{\hat{\mu}} = C_{\hat{\mu}}(\Omega)$ is a positive constant depending on $\hat{\mu}$ and Ω but independent of $\hat{\lambda}$. Gathering this latter result with the right hand side of (32), we end up with the estimate

$$\begin{aligned}
\|\Pi_h \tilde{\sigma} - \tilde{\sigma}_h\|_{0,\Omega} & \leq C(\|\sigma - \Pi_h \sigma\|_{0,\Omega} + \|p - s_h p\|_{0,\Omega} + \|\omega - \rho_h^{1,c} \omega\|_{0,\Omega}) \\
& \leq Ch(|\sigma|_{1,\Omega} + |p|_{1,\Omega} + |\omega|_{1,\Omega}),
\end{aligned} \tag{33}$$

where we have used the standard interpolation estimates for the quantities $\|\sigma - \Pi_h \sigma\|_{0,\Omega}$, $\|p - s_h p\|_{0,\Omega}$ and $\|\omega - \rho_h^{1,c} \omega\|_{0,\Omega}$. Moreover, the error equation (30) and the coerciveness of the bilinear form $c(\cdot, \cdot)$ yield, after some algebra, the following estimate

$$\|s_h p - p_h\|_{0,\Omega} \leq C(\|p - s_h p\|_{0,\Omega} + \|\sigma - \Pi_h \sigma\|_{0,\Omega}). \tag{34}$$

Relations (34) and (33), via triangle inequality, eventually lead to (23). We conclude the proof establishing (24) and (25). From the relation (26)₂, we have

$$b_1(\hat{P}_h \hat{u} - \hat{u}_h, \tilde{\tau}_h) = a(\tilde{\sigma}_h - \tilde{\sigma}, \tilde{\tau}_h) + b_1(\hat{P}_h \hat{u} - \hat{u}, \tilde{\tau}_h) + b_2(\tilde{u} - \tilde{u}_h, \tilde{\tau}_h) \quad \forall \tilde{\tau}_h \in \Sigma_h.$$

Observing that

$$b_1(\hat{P}_h \hat{u} - \hat{u}, \tilde{\tau}_h) = \int_{\Omega} (\rho_h^{1,c} \omega - \omega) a_s(\tilde{\tau}_h) dx \quad \forall \tilde{\tau}_h \in \Sigma_h,$$

using Proposition 1 and the standard interpolation estimates for the quantities $\|p - s_h p\|_{0,\Omega}$, $\|\sigma - \Pi_h \sigma\|_{0,\Omega}$ and $\|\omega - \rho_h^{1,c} \omega\|_{0,\Omega}$, we obtain

$$\|P_h^0 u - u_h\|_{0,\Omega} + \|\rho_h^{1,c} \omega - \omega_h\|_{0,\Omega} \leq Ch(|\sigma|_{1,\Omega} + |p|_{1,\Omega} + |\omega|_{1,\Omega}), \tag{35}$$

that, via triangle inequality, eventually leads to (24) and (25). \square

In the DMH approach, λ_h is an approximation of u on the edges of the triangulation. Our aim is thus to derive error bounds for $(u_{\partial K} - \lambda_h)$. In doing this

we will also obtain a sharper estimate on $\|P_h^0 u - u_h\|_{0,\Omega}$ than the one obtained in (35). To proceed, we first need to recall the following result [11]:

Lemma 3.2 *For all $T \in (W^{-1/q,q}(\partial K))^2$ there exists a unique $\tau_h \in \mathbb{D}(K)$ such that $\forall K \in \mathcal{T}_h$ we have*

$$\int_{\partial K} (\tau_h n - T) \cdot r_0 = 0 \quad \forall r_0 \in (R_0(\partial K))^2. \quad (36)$$

Furthermore, if \mathcal{T}_h is uniformly regular (see [9]), then there is a constant C independent of K such that

$$\|\tau_h\|_{0,K} \leq Ch^{2/p-1} \|T\|_{-1/q,q,\partial K}, \quad (37)$$

and

$$\|\operatorname{div} \tau_h\|_{0,K} \leq Ch^{2/p-2} \|T\|_{-1/q,q,\partial K}, \quad (38)$$

where p is defined as in (4), q is its conjugate and the norm $\|\cdot\|_{-1/q,q,\partial K}$ has been defined in (1).

We are now in a position to state the following result:

Theorem 3.2 *Let $(\tilde{\sigma}, \tilde{u})$ be the solution of problem (12) and $(\tilde{\sigma}_h, \tilde{u}_h)$ be the solution of problem (16). If the triangulation is uniformly regular and $\sigma \in (H^1(\Omega))^4$, $\operatorname{div} \sigma \in (H^1(\Omega))^2$, $p \in (H^1(\Omega) \cap L_0^2(\Omega))$ and $\omega \in H^1(\Omega)$, then there exists a constant C independent of h such that*

$$\|P_h^0 u - u_h\|_{0,\Omega} \leq Ch^2 (|\sigma|_{1,\Omega} + |p|_{1,\Omega} + |\operatorname{div} \sigma|_{1,\Omega} + |\omega|_{1,\Omega}), \quad (39)$$

$$\|\rho_h^0 \lambda - \lambda_h\|_{1/q,p,\partial K} \leq Ch^{2/p} (|\sigma|_{1,\Omega} + |p|_{1,\Omega} + |\operatorname{div} \sigma|_{1,\Omega} + |\omega|_{1,\Omega}) \quad \forall K \in \mathcal{T}_h, \quad (40)$$

where the norm $\|\cdot\|_{1/q,p,\partial K}$ has been defined in (2).

Proof. To prove (39) we use a duality argument (see [2]).

Define the pair $v \in H^2(\Omega)$ and $\tau \in \{\xi \in (H^1(\Omega))^4 \mid \operatorname{as}(\xi) = 0, \int_{\Omega} \operatorname{tr} \xi \, dx = 0\}$ as the solution of the elasticity system

$$\begin{cases} \tau = 2\hat{\mu}\epsilon(v) + \hat{\lambda}\operatorname{tr}(\epsilon(v))\delta & \text{in } \Omega, \\ \operatorname{div} \tau = P_h^0 u - u_h & \text{in } \Omega, \\ v = 0 & \text{on } \Gamma, \end{cases} \quad (41)$$

and set $\eta = (\operatorname{curl} v)/2$, $\zeta = -(\operatorname{tr} \tau)/2$. Since $(P_h^0 u - u_h) \in L^2(\Omega)$ and Ω is a convex polygon in \mathbb{R}^2 , we have the following a-priori estimate for the solution of (41)

$$\|\tau\|_{1,\Omega} + \|\zeta\|_{1,\Omega} + \|v\|_{2,\Omega} + \|\eta\|_{1,\Omega} \leq C \|P_h^0 u - u_h\|_{0,\Omega}. \quad (42)$$

Now,

$$\begin{aligned}
\|P_h^0 u - u_h\|_{0,\Omega}^2 &= \int_{\Omega} \operatorname{div} \tau (P_h^0 u - u_h) dx = \int_{\Omega} \operatorname{div} (\Pi_h \tau) (P_h^0 u - u_h) dx \\
&= a(\sigma_h - \sigma, \Pi_h \tau) + \int_{\Omega} (\omega_h - \omega) \operatorname{as}(\Pi_h \tau) dx + \int_{\Omega} \frac{\rho_{\widehat{\lambda}}}{2} (p_h - p) \operatorname{tr} (\Pi_h \tau) dx \\
&= a(\sigma_h - \sigma, \tau) + a(\sigma_h - \sigma, \Pi_h \tau - \tau) + \int_{\Omega} (\omega_h - \omega) \operatorname{as}(\Pi_h \tau - \tau) dx \quad (43) \\
&+ \int_{\Omega} \frac{\rho_{\widehat{\lambda}}}{2} (p_h - p) \operatorname{tr} (\Pi_h \tau - \tau) dx + \int_{\Omega} \frac{\rho_{\widehat{\lambda}}}{2} (p_h - p) \operatorname{tr} (\tau) dx \\
&= I_1 + I_2 + I_3 + I_4 + I_5.
\end{aligned}$$

It is immediate to deduce from (23),(25) and (42) that

$$|I_2| + |I_3| + |I_4| \leq Ch^2(|\sigma|_{1,\Omega} + |p|_{1,\Omega} + |\omega|_{1,\Omega}) \|P_h^0 u - u_h\|_{0,\Omega}. \quad (44)$$

To bound $I_1 + I_5$, we use the defining equations for τ, v, η and ζ and those for σ, σ_h and p, p_h to compute

$$\begin{aligned}
I_1 + I_5 &= \frac{1}{2\mu} \int_{\Omega} (\sigma_h - \sigma) : \tau dx + \int_{\Omega} \frac{\rho_{\widehat{\lambda}}}{2} (p_h - p) \operatorname{tr} (\tau) dx \\
&= \frac{1}{2\widehat{\mu}} \int_{\Omega} (\sigma_h - \sigma) : (\nabla v - \eta \chi) dx - \int_{\Omega} \rho_{\widehat{\lambda}} \left[\frac{1}{2} \operatorname{tr} (\sigma_h - \sigma) + (p_h - p) \right] \zeta dx \\
&= \frac{1}{2\widehat{\mu}} \int_{\Omega} \operatorname{div} (\Pi_h \sigma - \sigma) (v - P_h^0 v) dx - \int_{\Omega} (\eta - \rho_h^{1,c} \eta) \operatorname{as}(\Pi_h \sigma - \sigma) dx \\
&- \int_{\Omega} \rho_{\widehat{\lambda}} \left[\frac{1}{2} \operatorname{tr} (\sigma_h - \sigma) + (p_h - p) \right] (\zeta - s_h \zeta) dx,
\end{aligned}$$

so that

$$|I_1| + |I_5| \leq Ch^2(|\sigma|_{1,\Omega} + |\operatorname{div} \sigma|_{1,\Omega} + |p|_{1,\Omega} + |\omega|_{1,\Omega}) \|P_h^0 u - u_h\|_{0,\Omega}. \quad (45)$$

Combining (43),(44) and (45), we obtain (39).

To obtain (40), we let τ be any element of $(W_q(\operatorname{div}; K))^2$ and $\bar{\tau}_h \in \mathbb{D}(K)$ be defined by (36) with $T = \tau n|_{\partial K}$ and we take $\tilde{\tau}_h \equiv \tau_h$ such that

$$\tau_h|_K = \bar{\tau}_h, \quad \tau_h|_{K'} = 0, \quad \forall K' \neq K, \quad \forall K \in \mathcal{T}_h,$$

thus obtaining from the first equation of (12) and the first equation of (16)

$$\begin{aligned}
\int_{\partial K} \bar{\tau}_h \cdot n (\lambda - \lambda_h) ds &= \frac{1}{2\widehat{\mu}} \int_K (\sigma - \sigma_h) \bar{\tau}_h dx + \int_K (u - u_h) \operatorname{div} (\bar{\tau}_h) dx \\
&+ \int_K (\omega - \omega_h) \operatorname{as}(\bar{\tau}_h) dx + \frac{\rho_{\widehat{\lambda}}}{2} \int_K (p - p_h) \operatorname{tr} (\bar{\tau}_h) dx,
\end{aligned}$$

which can be written as

$$\begin{aligned} \int_{\partial K} \bar{\tau} \cdot n (\rho_h^0 \lambda - \lambda_h) ds &= \frac{1}{2\hat{\mu}} \int_K (\sigma - \sigma_h) \bar{\tau}_h dx + \int_K (P_h^0 u - u_h) \operatorname{div}(\bar{\tau}_h) dx \\ &+ \int_K (\omega - \omega_h) \operatorname{as}(\bar{\tau}_h) dx + \frac{\rho_{\hat{\lambda}}}{2} \int_K (p - p_h) \operatorname{tr}(\bar{\tau}_h) dx. \end{aligned}$$

Owing to the definition of $\bar{\tau}_h$, using (37) and the definition (2) (38) and (39), we eventually get

$$\|\rho_h^0 \lambda - \lambda_h\|_{1/q,p,\partial K} \leq Ch^{2/p} (|\sigma|_{1,\Omega} + |p|_{1,\Omega} + |\operatorname{div} \sigma|_{1,\Omega} + |\omega|_{1,\Omega}) \quad \forall K \in \mathcal{T}_h.$$

Since $p < 2$, estimate (40) can be regarded as a superconvergence property for λ_h . In practical computations, we shall demonstrate the superconvergence of λ_h using a different norm more easily computable than (2), as suggested in [1]. \square

4 Modeling of the thermal oxidation process in semiconductor technology

Thermal oxidation is one of the several steps involved in the manufacturing of integrated circuits. The numerical simulation of this process is aimed at predicting the final shape of the oxidized structure in order to assess the electrical and mechanical performance of the semiconductor device. In this section we present a brief description of the thermal oxidation process and we give some details about its mathematical and numerical modeling using the DMH discretization (for a more comprehensive mathematical model of the thermal oxidation process, we refer to the recent work [22]).

The oxidation process is a complex phenomenon where a layer of oxide (SiO_2), that is usually employed as an electric insulator, is thermally grown on a silicon wafer bulk (Si). The surface of the Si is masked by a silicon-nitride (Si_3N_4) pattern impermeable to the oxidant penetration and is exposed to oxygen or water vapor at high temperature for a certain oxidation time (generally, 1-2 hours). The oxygen diffuses through the oxide and reacts with the silicon at the Si-SiO_2 interface. Since the SiO_2 has a molar volume 2.2 times greater than the Si , at each time of the process a volume fraction of the new grown oxide replaces the silicon that has been consumed, while the remaining volume fraction pushes the old oxide upward. This constrained volume expansion gives rise to large stresses and in particular causes the SiO_2 to undergo a compression state and the Si to undergo a tension state. Experimental evidence [20,6] shows that this state of stress can significantly affect both the O_2 diffusion in the pre-existing SiO_2 layer and also the chemical reaction kinetics between the O_2 and the Si . The combination of these effects determines the final shape

of the Si-SiO₂ system, that in turn can considerably affect the overall electric performance of the semiconductor device and its mechanical reliability. A schematic representation of the thermal oxidation process is shown in Fig.2.

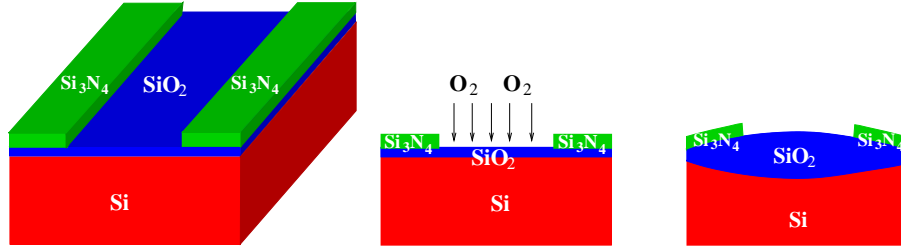


Figure 2. Schematics of the thermal oxidation process in a local oxidation structure (LOCOS): 3D model (left), 2D reduction (center) at the beginning of the oxidation and 2D model (left) after process completion.

The mathematical model of the process considers a sequence of quasi-stationary steps each involving the solution of two groups of PDEs systems over a domain whose shape changes with time. The two PDE systems are mutually dependent: the diffusion and kinetic reaction coefficients as well as the geometry of the deformed domain depend on the stress distribution; in turn, the chemical reaction forces the oxide-silicon interface to move, driving the mechanical problem. After solving the diffusion-reaction problem, an incremental stress analysis is performed on the structure to compute the new stress field and the resulting deformed configuration (see Fig.3). Notice how the data exchanged

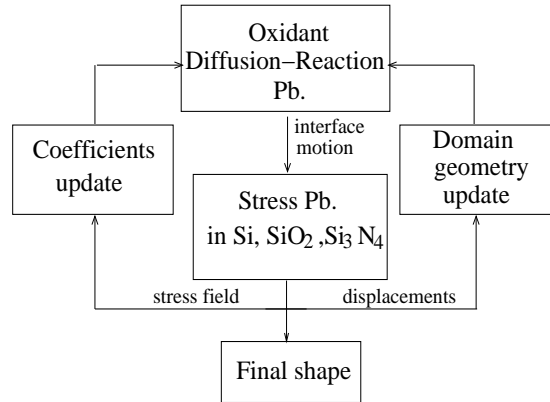


Figure 3. Flux diagram for the thermal oxidation process simulation.

between the sub-blocks in both the coupled systems are stress dependent quantities, so that the quality of their approximation clearly affects the accuracy of the overall computation. In a standard displacement finite element approach, fluxes and stresses are typically post-processed quantities that suffer from a number of limitations such as the failure of the post-processed stresses at satisfying self-equilibrium and interelement traction reciprocity, and the possible onset of locking problems in the incompressible regime. The DMH approach is specifically tailored to overcome these limitations with a computational cost

not severely exceeding the one of standard displacement methods applied to the solution of the problem at hand.

4.1 Fluid-mechanical model for the thermal oxidation process

There are several models to describe the stress field evolution during the oxidation process, some of which are very advanced. In any case, it is commonly accepted that different continuum-mechanics models need to be adopted to describe faithfully the mechanical behavior of each material involved in the oxidation process. Following the experiments of [6] and [20], the Si_3N_4 stripe and the Si bulk have been modeled in this work as linear isotropic elastic materials, while a non-Newtonian model is used for the SiO_2 . Precisely, the SiO_2 is represented by an incompressible non-Newtonian fluid with nonlinear viscosity of Eyring type

$$\mu(\sigma) = \mu_0 \frac{\tau_{max}/\sigma_c}{\sinh(\tau_{max}/\sigma_c)}, \quad \tau_{max} = \sqrt{\frac{(\sigma_{11} - \sigma_{22})^2}{4} + \sigma_{12}^2},$$

where μ_0 is the stress-free constant viscosity, τ_{max} is a critical stress value and $\sigma_c = 2k_B T/V_c$, V_c being an activation volume, k_B the Boltzmann constant and T the temperature of the process (isothermal conditions are supposed).

From the above discussion, it turns out that the problem at hand involves materials with heterogeneous fluid-mechanical properties, leading to a fluid-structure interaction problem. In particular, the interaction between the Si domain and the SiO_2 - Si_3N_4 domains is handled by a standard Boundary Loading Method, since it can be checked that the deformations produced by the Si domain on the SiO_2 are negligible. The interaction between the SiO_2 and the Si_3N_4 domains is instead handled by a coupled procedure, with an inner iterative map to solve for the nonlinear dependence of the oxide viscosity on the normal stresses. Notice that this coupling procedure is easily implemented due to the use of the unified compressible/incompressible formulation of the DMH method, the only difference being in the numerical values of the Lamè parameters in the two subdomains.

5 Numerical results

In this section we first present some numerical results concerning the fluid-mechanical problem and then we validate the DMH formulation on a realistic simulation of a LOCOS device. Mixed Dirichlet-Neumann boundary conditions will be considered in all the numerical experiments.

The dual mixed-hybrid method has been tested in the case of compressible elastic problems and incompressible fluid problems. In the first example a vertical compressive load of 100 Nm^{-2} is applied to a $(1 \times 3) \text{ m}$ rectangular plate along the portion $x \in [1.5, 2]$ of the upper edge. The plate is clamped along the vertical edges, is stress-free along the bottom edge and is constituted by two materials with Young modulus $E_1 \ll E_2$, with $E_1 = 2 \cdot 10^4 \text{ Pa}$ and $E_2 = 2 \cdot 10^5 \text{ Pa}$, respectively. In Fig.4 we show the deformations and the stresses due to the load when the two materials are vertically stratified. Looking at the stress distribution, we clearly see that the applied load is much more consistently transferred from the material on the top to the material on the bottom when the softer material is situated over the stiffer material (Fig.4, rightmost column). This latter situation is somewhat similar to the situation occurring in the oxidation problem, where a structure made of materials with different stiffness properties is subjected to a force field.

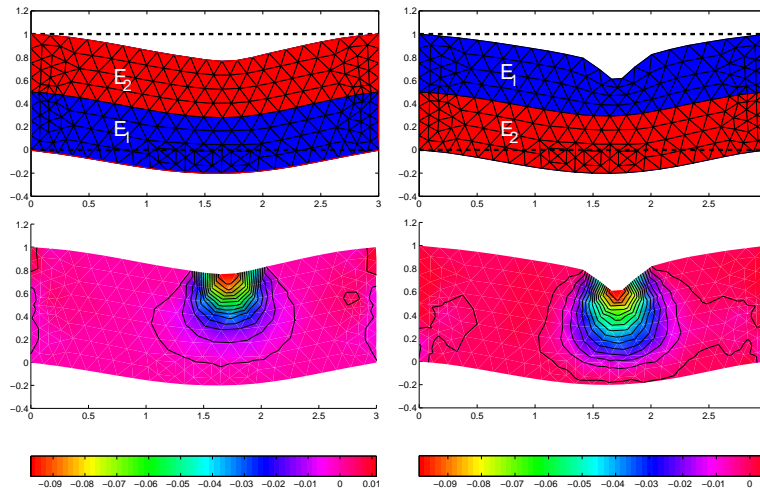


Figure 4. Deformations (here amplified by a factor 100 for graphical purposes) of a rectangular plate constituted of materials with stiffness $E_2 \gg E_1$ subject to a compressive load (top row) and σ_{22} component of the stress (bottom row).

As a second test case, we show the results for a simple fluid-elastic interacting structure solved using the unified coupled procedure discussed in the previous section. The domain Ω is the unit square, with the upper half behaving like a fluid, while the lower half behaving like an elastic solid (with a very low Young modulus). For a certain time interval a compressive load is applied on the top edge of the fluid domain, while stress-free boundary conditions and null displacements are assumed on the vertical and bottom sides, respectively for all the time duration of the simulation. At a certain time, the load is released and the elastic solid relaxes recovering its original shape and squeezing out the fluid, as shown in Fig.5 where some phases of the temporal evolution of

the phenomenon are displayed.

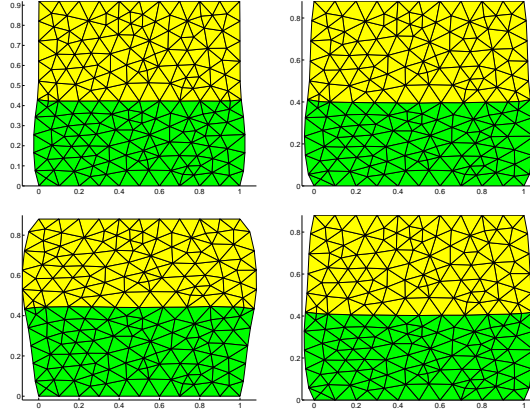


Figure 5. Temporal evolution of the coupled fluid-elastic interacting system. The four diagrams must be looked at in clockwise rotation sequence from top left position.

Finally, we assess numerically the convergence properties of the DMH formulation solving the Stokes problem for an incompressible fluid squeezed between two parallel plates moving one toward the other with constant velocity (see [24] for the analytical solution of the problem). Due to the symmetry of the problem, the computation has been carried out only on a quarter of the domain, that is the dashed-line region in Fig.6. Symmetry boundary conditions have been enforced on the left and bottom edges as shown in Fig.6. Observe that in the DMH formulation Neumann boundary conditions are imposed on the complete stress tensor, unlike in displacement-based formulations, where the same boundary condition is enforced on the tensor $\nu \nabla u - p \delta$, this latter procedure being variationally correct but not physically consistent (see *e.g.* [19], Sect.10.1.1).

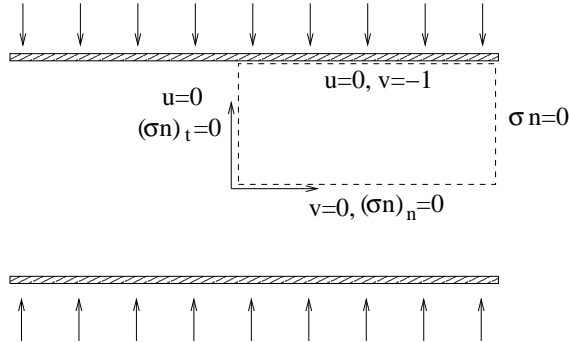


Figure 6. Geometry of the domain and boundary conditions for the Stokes problem.

The computed error curves are in agreement with the theoretical estimates given in Sect.3. Observe in particular the superconvergence of λ_h measured in

the norm

$$\|\lambda_h\|_{\mathcal{E}_h} = \left(\sum_{e \in \mathcal{E}_h} |e| \|\lambda_h\|_{(L^2(e))^2}^2 \right)^{1/2}, \lambda_h \in \Lambda_h$$

(see [1] and [5], Ch.5, p.188). This norm is standard in the error analysis of hybridized mixed finite element methods and can be regarded as a practically feasible numerical implementation of the (sharper) norm $\|\cdot\|_{1/q,p,\partial K}$ used in the theoretical error analysis.

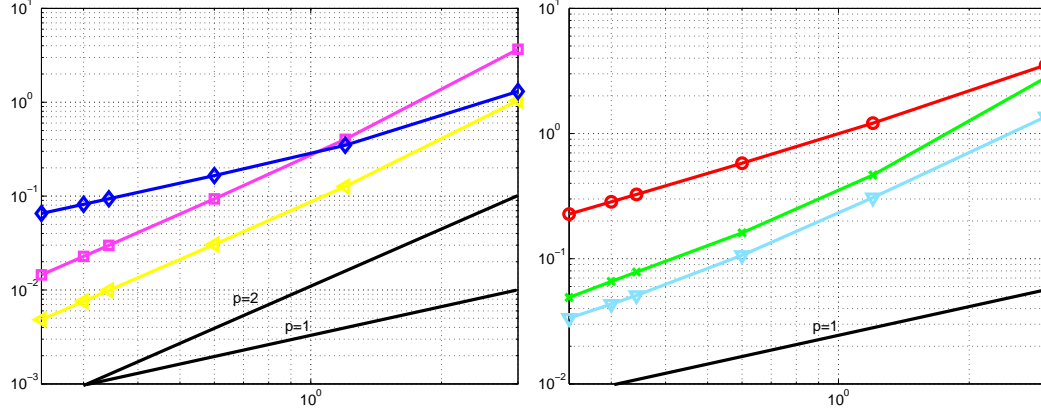


Figure 7. Error norms. On the left: $\|u - u_h\|_{(0,\Omega)}$ (\diamond), $\|\rho_h^0 u - \lambda_h\|_{\mathcal{E}_h}$ (\square), $\|P_h u_h - u_h\|_{(0,\Omega)}$ (∇). On the right: $\|\sigma - \sigma_h\|_{(0,\Omega)}$ (\circ), $\|p - p_h\|_{(0,\Omega)}$ (∇), $\|\omega - \omega_h\|_{(0,\Omega)}$ (\times).

5.2 Thermal oxidation simulation

We have considered a computational domain that is one half of the local oxidation structure shown in Fig.2. The total oxidation time considered in this simulation is 1500s. The device has semi-length 1.5 $m\mu$, is padded with an oxide layer initially 0.015 $m\mu$ thick and is patterned with a 0.75 $m\mu$ thick nitride mask. Material properties have been chosen as in [22]. In Fig.8 the deformed configuration and the corresponding pressure field are shown at different time levels. The typical "bird's beak" shape of the final oxide configuration is clearly recognizable. The largest stresses arise as expected on the junction line between the SiO_2 and the Si_3N_4 regions and in particular near the rightmost edge of the Si_3N_4 band.

6 Conclusions and future work

In this paper we have presented and theoretically analyzed a dual-mixed hybrid (DMH) formulation capable of treating in a unified framework both compressible and incompressible problems in continuum mechanics. This allows

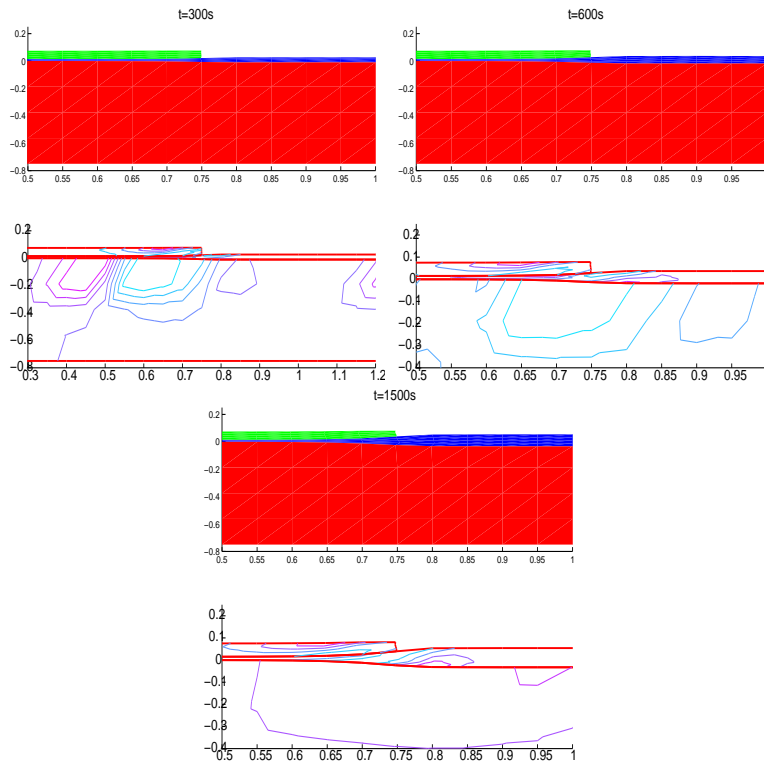


Figure 8. Deformed configuration (top, zoom of the area) and pressure field (bottom) for $t = 300, 600, 1500$ s.

for handling in a simple and efficient manner problems with different materials using a unique computer code. The DMH approach has been employed in the computation of the stress field in the simulation of the thermal oxidation process in semiconductor technology. In this application it is necessary to compute accurately the stress field both in an incompressible fluid (SiO_2) and in elastic solids ($\text{Si}_3\text{N}_4, \text{Si}$). In particular, the Si_3N_4 - SiO_2 domains have been considered as a unique material with different Lamè parameters. The results show the accuracy and the flexibility of the method.

The future research will consist in implementing several improvements of the present model. In particular it is planned to:

- i) adopt a more realistic solid viscoelastic model for the Si_3N_4 ;
- ii) account for the monocrystalline structure of the Si by adopting an anisotropic elastic model. In this respect, the DMH formulation has been recently extended in [8] to deal with orthotropic materials, which covers the standard crystalline configurations used in semiconductor device technology.

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