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Simulating Squeeze Flows in Multiaxial Laminates using an improved TIF model

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Abstract. Thermoplastic composites are widely considered in structural parts. In this paper attention is paid to squeeze flow of continuous fiber laminates. In the case of unidirectional prepregs, the ply constitutive equation is modeled as a transversally isotropic fluid, that must satisfy both the fiber inextensibility as well as the fluid incompressibility. When laminate is squeezed the flow kinematics exhibits a complex dependency along the laminate thickness requiring a detailed velocity description through the thickness. In a former work the solution making use of an in-plane-out-of-plane separated representation within the PGD – Poper Generalized Decomposition – framework was successfully accomplished when both kinematic constraints (inextensibility and incompressibility) were introduced using a penalty formulation for circumventing the LBB constraints. However, such a formulation makes difficult the calculation on fiber tractions and compression forces, the last required in rheological characterizations. In this paper the former penalty formulation is substituted by a mixed formulation that makes use of two Lagrange multipliers, while addressing the LBB stability conditions within the separated representation framework, questions never until now addressed.

INTRODUCTION

Thermoplastic composites are preferred structural materials due to their excellent damage tolerance properties, shorter manufacturing cycles and ease of weldability. One of the precursor material to fabricate thermoplastic composite parts is an unidirectional (UD) prepreg which consists of aligned continuous fibers pre-impregnated with thermoplastic resin. In their melt state, UD prepreg can be viewed as inextensible fibers surrounded by an incompressible viscous matrix, and hence can be modeled as a transversally isotropic fluid [7, 16]. These UD laminates are usually stacked in desired orientations to create a composite laminate.

Applied pressures during processing induce laminate deformation consisting of either squeeze flow of the matrix and fiber together or flow of the melt polymer through the fiber network. The squeeze flow behaviour of both unidirectional and multiaxial laminates has been studied in [12, 2, 11, 14, 15, 10, 3]. Due to the high viscosity of thermoplastic matrix and high fiber content of UD prepregs, the dominant material deformation occurs due to the squeeze flow.

The squeeze flow behaviour of both unidirectional and multiaxial laminates has been studied using a high-resolution numerical strategy in our former work [9], where a penalty formulation of the Ericksen fluid flow using an in-plane-out-of-plane separated representation. Such separated representation was introduced and successfully applied for addressing problems defined in degenerated domains in which at least one of its characteristic dimensions is much smaller than the others. This is the case of laminates in which rich behaviors can occur in the thickness direction, needing for a fully 3D discretization. In that circumstances standard mesh-based discretization fail to address a rich enough out-of-plane representation. The use of an in-plane-out-of-plane separated representation makes possible to separate during the problem resolution the in-plane and out-of-plane problems allowing a extremely rich representation of 3D behaviors while keeping the computational complexity 2D (the one associated to the in-plane problem being the out-of-plane problem one-dimensional). This separated representation was considered in our former works [1, 5, 4, 6, 8].

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In [13] a penalty and mixed formulations of the Stokes flow in a narrow gap, easily generalized to stratified flows was successfully considered and extended for addressing the flow of multi axial laminates making use of the Ericksen fluid flow model at the ply level. In this last case the penalty formulation related to both the fiber inextensibility and the flow incompressibility considered in [9] is substituted in favor of a mixed formulation making use of two Lagrange multipliers, the first related to the inextensibility constraint and the second one to the flow incompressibility. Such a richer description is needed to evaluate the fiber tension, crucial to predict defects related to its compression. On the other hand the rheological characterization of multiaxial laminates is performed by calculating the compression force to be applied for obtaining a given squeeze rate. For that purpose, it is important calculating the stress tensor in the fluid, and when using a penalty formulation the calculation of the pressure field remains a tricky issue. These facts justify the use of a mixed formulation instead of the penalized one previously considered in our former works, formulation that was retained in [9] for circumventing the issues related to the LBB stability condition. However in [13] an issue was found when addressing multiaxial laminates composed of TIF layers. A singularity in the fiber tension was found at the plies interfaces. In the present work we propose an alternative modeling able to circumvent the just referred issue.

NUMERICAL SOLVER BASED ON SEPARATED REPRESENTATIONS

In-plane-out-of-plane separated representation

The in-plane-out-of-plane separated representation allows the solution of full 3D models defined in plate geometries with a computational complexity characteristic of 2D simulations. This separated representation allows independent representations of the in-plane and the thickness fields dependencies. The main idea lies in the separated representation of the velocity field by using functions depending on the in-plane coordinates $\mathbf{x} = (x, y)$, $\mathbf{P}_i^j(\mathbf{x})$, and others depending on the thickness direction z, $\mathbf{T}_i^j(z)$, according to:

$$\begin{pmatrix} \mathbf{v}(\mathbf{x}, z) \\ p(\mathbf{x}, z) \end{pmatrix} = \begin{pmatrix} u(\mathbf{x}, z) \\ v(\mathbf{x}, z) \\ w(\mathbf{x}, z) \\ p(\mathbf{x}, z) \end{pmatrix} \approx \begin{pmatrix} \sum_{i=1}^{N} P_i^1(\mathbf{x}) \cdot T_i^1(z) \\ \sum_{i=1}^{N} P_i^2(\mathbf{x}) \cdot T_i^2(z) \\ \sum_{i=1}^{N} P_i^3(\mathbf{x}) \cdot T_i^3(z) \\ \sum_{i=1}^{N} P_i^p(\mathbf{x}) \cdot T_i^p(z) \end{pmatrix} = \sum_{i=1}^{N} \mathbf{P}_i(\mathbf{x}) \circ \mathbf{T}_i(z), \tag{1}$$

where ”∘” denotes the entry-wise or Hadamard’s product.

Using this notation in (1), the velocity gradient $\nabla\mathbf{v}(\mathbf{x}, z)$ can be written as

$$\nabla\mathbf{v} = \sum_{i=1}^{N} \mathbb{P}_i(\mathbf{x}) \circ \mathbb{T}_i(z) \tag{2}$$

with matrices $\mathbb{P}_i$ and $\mathbb{T}_i$ defined in [13].

Flow model

The Stokes flow model is defined in $\Xi = \Omega \times \mathcal{I}$, $\Omega \subset \mathbb{R}^2$ and $\mathcal{I} \subset \mathbb{R}$, and for an incompressible fluid, in absence of inertia and mass terms reduces to:

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma} = -p\mathbf{I} + 2\eta\mathbf{D} \\ \nabla \cdot \mathbf{v} = 0 \end{cases}, \tag{3}$$

where $\boldsymbol{\sigma}$ is the Cauchy’s stress tensor, $\mathbf{I}$ the unit tensor, η the fluid viscosity, p the pressure (Lagrange multiplier associated with the incompressibility constraint) and the rate of strain tensor $\mathbf{D}$ being the symmetric component of the velocity gradient.

The weak form of the coupled velocity-pressure Stokes problem, for both a test velocity $\mathbf{v}^*$ and a test pressure $\mathbf{p}^*$, the first vanishing on the boundary in which the velocity is prescribed, and assuming null tractions in the remaining part of the domain boundary, can be written as

$$\int_{\Omega \times \mathcal{I}} \left(-p\mathrm{Tr}(\mathbf{D}^*) + 2\eta \mathbf{D}^* : \mathbf{D}\right) \, d\mathbf{x} \, dz = 0, \tag{4}$$

$$\int_{\Omega \times \mathcal{I}} -p^* \mathrm{Tr}(\mathbf{D}) \, d\mathbf{x} \, dz = 0, \tag{5}$$

where Eqs. (4) and (5) make reference to the linear momentum and mass balances respectively. The weak form separated representation was fully defined in [13].

Separated representation constructor

The construction of the solution separated representation is performed incrementally, a term of the sum at each iteration. Thus, supposing that at iteration $n-1$, $n \geq 1$ and $n \leq N$, the first $n-1$ terms of both velocity and pressure separated representations were already computed

$$\mathbf{v}^{n-1}(\mathbf{x}, z) = \sum_{i=1}^{n-1} \mathbf{P}_i^v(\mathbf{x}) \circ \mathbf{T}_i^v(z) \;\; \& \;\; p^{n-1}(\mathbf{x}, z) = \sum_{i=1}^{n-1} P_i^p(\mathbf{x}) \cdot T_i^p(z), \tag{6}$$

and the improved velocity field $\mathbf{v}^n(\mathbf{x}, z)$ at iteration n reads

$$\mathbf{v}^n(\mathbf{x}, z) = \sum_{i=1}^{n} \mathbf{P}_i^v(\mathbf{x}) \circ \mathbf{T}_i^v(z) = \mathbf{v}^{n-1}(\mathbf{x}, z) + \mathbf{P}_n^v(\mathbf{x}) \circ \mathbf{T}_n^v(z), \tag{7}$$

and similarly for the improved pressure field $p^n(\mathbf{x}, z)$ at iteration n

$$p^n(\mathbf{x}, z) = \sum_{i=1}^{n} P_i^p(\mathbf{x}) \cdot T_i^p(z) = p^{n-1}(\mathbf{x}, z) + P_n^p(\mathbf{x}) \cdot T_n^p(z). \tag{8}$$

By introducing these expressions making use of the separated representation into the Stokes' problem weak form and proceeding as indicated in [13] both the updated velocity and updated pressure fields at iteration n are calculated.

Flow in a laminate

Consider a laminate composed of $\mathcal{P}$ layers in which each layer involves a linear and isotropic viscous fluid of viscosity η_i, thus the extended Stokes flow problem in its weak form involves the dependence of the viscosity along the thickness direction.

If H is the total laminate thickness, and assuming for the sake of simplicity and without loss of generality that all the plies have the same thickness h, it results $h = \frac{H}{\mathcal{P}}$. Now, from the characteristic function of each ply $\chi_i(z)$, $i = 1, \cdots, \mathcal{P}$:

$$\chi_i(z) = \begin{cases} 1 & \text{if } (i-1)h \leq z < ih \\ 0 & \text{elsewehere} \end{cases}, \tag{9}$$

the viscosity reads

$$\eta(\mathbf{x}, z) = \sum_{i=1}^{\mathcal{P}} \eta_i \cdot \chi_i(z), \tag{10}$$

where it is assumed, again without loss of generality, that the viscosity does not evolve in the plane, i.e. $\eta_i(\mathbf{x}) = \eta_i$.

This decomposition is fully compatible with the velocity-pressure separated representation (1).

Ericksen fluid flow model in a laminate

The case of a prepreg ply reinforced by continuous fibres oriented along direction $\mathbf{p}^T = (p_x, p_y, 0)$, $\|\mathbf{p}\| = 1$, is analyzed here. It is assumed that the thermoplastic resin exhibits Newtonian behaviour. Thus the velocity $\mathbf{v}(\mathbf{x}, z)$ of the equivalent anisotropic fluid must satisfy the incompressibility and inextensibility constraints

$$\nabla \cdot \mathbf{v} = 0, \tag{11}$$

and

$$\mathbf{p}^T \cdot \nabla\mathbf{v} \cdot \mathbf{p} = 0, \tag{12}$$

respectively. Expression (12) can be rewritten using tensor notation as $\nabla\mathbf{v} : \mathbf{a} = 0$, where the second order orientation tensor $\mathbf{a}$ is defined from $\mathbf{a} = \mathbf{p} \cdot \mathbf{p}^T = \mathbf{p} \otimes \mathbf{p}$.

The orientation tensor $\mathbf{a}$ has only planar components (the out-of-plane fiber orientation can be neglected in the case of laminates), it is symmetric and of unit trace, i.e.

$$\mathbf{a} = \begin{pmatrix} a_{xx} & a_{xy} & 0 \\ a_{yx} & a_{yy} & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \mathcal{A} & \mathbf{0} \\ \mathbf{0}^T & 0 \end{pmatrix}, \tag{13}$$

where $\mathcal{A}$ represents the plane component of the orientation tensor $\mathbf{a}$, $a_{xy} = a_{yx}$ (i.e. $\mathcal{A} = \mathcal{A}^T$) and $a_{yy} = 1 - a_{xx}$.

The simplest expression of the Ericksen's constitutive equation [7] can be written in the compact form as follows

$$\boldsymbol{\sigma} = -p\mathbf{I} + \tau\mathbf{a} + 2\eta_T\mathbf{D} + 2(\eta_L - \eta_T)(\mathbf{D} \cdot \mathbf{a} + \mathbf{a} \cdot \mathbf{D}), \tag{14}$$

that is then introduced into the linear momentum balance

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}. \tag{15}$$

In Eq. (14) p and τ represents respectively the Lagrange multipliers related to the incompressibility and inextensibility constraints, and η_L and η_T the longitudinal and transverse shear viscosities respectively.

By separating both the pressure and the fiber tension fields using an in-plane-out-of-plane-separated representation

$$p(\mathbf{x}, z) = \sum_{i=1}^{N} P_i^p(\mathbf{x}) \cdot T_i^p(z), \tag{16}$$

and

$$\tau(\mathbf{x}, z) = \sum_{i=1}^{N} P_i^\tau(\mathbf{x}) \cdot T_i^\tau(z), \tag{17}$$

it allows accurate calculations of both the fiber tension and the pressure field. This information can be used to predict either fibers buckling or forces acting on the squeezed boundary.

The weak form for a test velocity $\mathbf{v}^*(\mathbf{x}, z)$ vanishing at the boundary in which velocity is prescribed, a test pressure $p^*(\mathbf{x}, z)$ and a test fiber tension $\tau^*(\mathbf{x}, z)$, assuming null tractions in the remaining part of the domain boundary can be expressed as

$$\int_{\Omega\times\mathcal{I}} \mathbf{D}^* : \boldsymbol{\sigma}\, d\mathbf{x}\, dz = 0, \quad \int_{\Omega\times\mathcal{I}} p^*\mathbf{D} : \mathbf{I}\, d\mathbf{x}\, dz = 0 \;\; \& \quad \int_{\Omega\times\mathcal{I}} \tau^*\mathbf{D} : \mathbf{a}\, d\mathbf{x}\, dz = 0. \tag{18}$$

PENALIZED VERSUS MIXED FORMULATIONS

Fully penalized formulation

Both Stokes and Ericksen flows have been successfully implemented by means of penalized formulations involving both, the pressure, p, and the fiber tension, τ. Such a penalized formulation leads to a problem that only involves the velocity field. Therefore, the aim is to clarify how the constitutive equation is modified when introducing two penalty parameters. For that purpose we consider:

$$\nabla \cdot \mathbf{v} + \lambda p = \mathbf{D} : \mathbf{I} + \lambda p = 0 \;\;\&\;\; \mathbf{D} : \mathbf{a} - \epsilon \tau = 0. \tag{19}$$

Where the coefficients λ and ϵ are chosen close to zero to ensure numerically incompressibility and fiber inextensibility. Both constraints are ensured as long as both penalty coefficients are small enough. Isolating p and τ from Eq. (19), it results

$$p = -\frac{1}{\lambda}\mathbf{D} : \mathbf{I} \;\;\&\;\; \tau = \frac{1}{\epsilon}\mathbf{D} : \mathbf{a}. \tag{20}$$

If both pressure and fiber tension are penalized the constitutive equation reduces to,

$$\boldsymbol{\sigma} = \frac{1}{\lambda}(\mathbf{I} \otimes \mathbf{I}) : \mathbf{D} + \frac{1}{\epsilon}(\mathbf{a} \otimes \mathbf{a}) : \mathbf{D} + 2\eta\mathbf{D}, \tag{21}$$

where a very high effective viscosity acts along the fiber direction. This formulation was intensively considered in [9] where a variety of results were presented and discussed, proving the potentiality of the approach. However neither fiber tension nor the pressure field were calculated because the penalty formulation does not allow an accurate post-calculation from the calculated velocity field and the penalty definitions (20).

Mixed formulation

The main issue when considering mixed formulation is the appropriate choice of functional spaces. In [13] a detailed analysis was conducted and the conclusions, supported by numerous numerical experiments, were quite simple: the functional spaces considered in both the in-plane and the out-of-plane approximation must ensure standard LBB conditions. Thus considering Q2/Q1/Q1 (for the velocity, pressure and tension respectively) in both approximations allows ensuring the stability requirements.

However, as soon as multiaxial laminates were addressed tension singularities appeared at the plies interfaces level, provocation a tension pic that perturbed the solution of both pressure ans fiber tension fields. The origin of the tension peak is easy to understand. The parabolic profile of $u(\mathbf{x}, z)$ through the ply thickness z in the upper ply implies a shear rate and consequently a shear stress at the interface. However, at the interface the x-component of the traction $\mathbf{T} = \boldsymbol{\sigma} \cdot \mathbf{e}_z$ ($\mathbf{e}_z$ being the unit vector defining the z-coordinate axis) computed at the bottom ply for equilibrating the shear stress associated to the parabolic profile in the upper-ply implies a non-null component xz of the rate of strain tensor, i.e. $\mathbf{D}_{xz} \neq 0$ (note that fiber tension τ is not involved in the expression of traction $\mathbf{T}$). Thus the u velocity in the bottom ply cannot be exactly zero, there is a boundary layer located at the interface in which it activates the fiber tension. Because as just indicated the fibers tension do not communicate along the thickness, the tension singularity remains located at the interface level and does not propagate in the bottom ply. The same reasoning applies for the parabolic profile of $v(\mathbf{x}, z)$ in the bottom ply that implies a tension singularity in the upper ply at the interface neighborhood. By diminishing the viscosity the shear stress decreases and then the tension peaks. This tendency has been verified numerically.

Solving the same problem by using an in-plane-out-of-plane separated representation seems a tricky issue because the inevitable singularity that the Ericksen model induces at the plies interface when the orientation of fibers evolves from one ply to its contiguous one. For this reason we finally decided in [13] to consider a velocity-pressure mixed formulation whereas the tension is treated from a penalty formulation. However, a way of circumventing such issue consists of adding an anisotropic viscosity such that the viscous stress term $\boldsymbol{\sigma}^v$ will write

$$\boldsymbol{\sigma}^v = 2\eta_T\mathbf{D} + \frac{2\eta_T}{\epsilon}\left[(\mathbf{p} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{p}) : \mathbf{D}\right](\mathbf{p} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{p}), \tag{22}$$

with ϵ small enough to avoid the tension singularity as proved in Fig. 1. The TFI model (14) with the anisotropic viscosity contribution (22) constitutes an improved TIF model particularly suitable for addressing 3D laminate models.

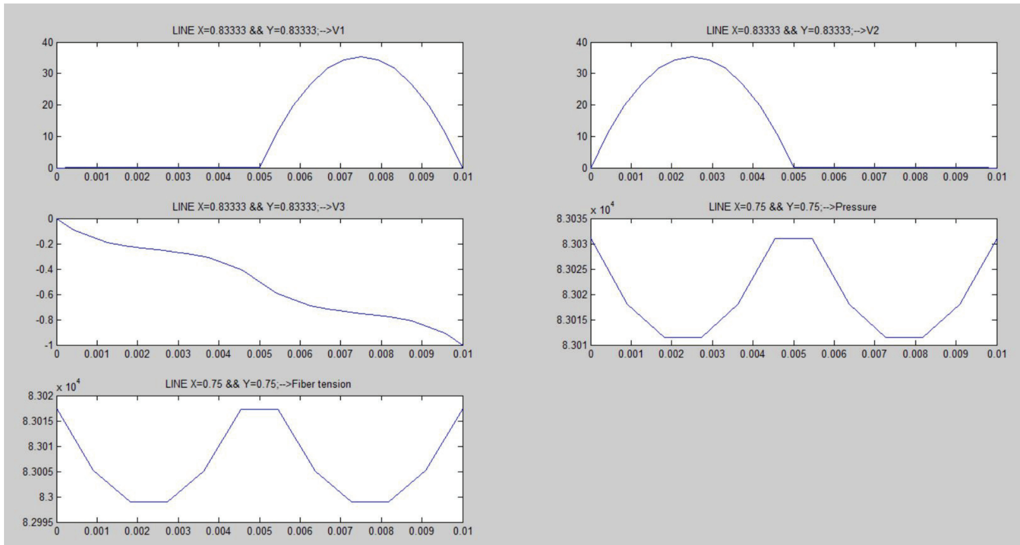

FIGURE 1. Mechanical problem and loading trajectory

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