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Advanced simulation of models defined in plate geometries: 3D solutions with 2D computational complexity

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ABSTRACT

Many models in polymer processing and composites manufacturing are defined in degenerated three-dimensional domains, involving plate or shell geometries. The reduction of models from 3D to 2D is not obvious when complex physics are involved. The hypotheses to be introduced for reaching this dimensionality reduction are sometimes unclear, and most of possible proposals will have a narrow interval of validity. The only getaway is to explore new discretization strategies able to circumvent or at least alleviate the drawbacks related to mesh-based discretizations of fully 3D models defined in plate or shell domains. An in-plane–out-of-plane separated representation of the involved fields within the context of the Proper Generalized Decomposition allows solving the fully 3D model by keeping a 2D characteristic computational complexity. Moreover the PGD features allow the introduction of many extra-coordinates, as for example the orientation of the different laminate plies, without affecting the solvability of the resulting multidimensional model.

1. Introduction

Many models in polymer processing and composites manufacturing are defined in degenerated three-dimensional domains. By degenerated we understand that at least one of the characteristic dimensions of the domain is much lower than the other ones. This situation is particularly common in models defined plate or shells type geometries.

Mesh based solutions of models defined in such degenerated domains is a challenging issue because the resulting meshes usually involve too many degrees of freedom. In that case the first question concerns the possibility of reducing the model complexity. Classical beam, plate or shell theories are some examples of simplified modeling where the 3D subjacent elastic model is substituted by lower dimensional models (1D in the case of beam theory and 2D in the case of plate and shell theories).

Going from a 3D elastic problem to a 2D plate theory model usually involves some kinematical and/or mechanical hypotheses [19] on the evolution of the solution through the thickness of the plate. Despite the quality of existing plate theories, their solution close to the plate edges is usually wrong as the displacement fields are truly 3D in those regions and do not satisfy the kinematic hypothesis. Indeed, the kinematic hypothesis is a good approximation where Saint-Venant's principle is verified. However, some heterogeneous complex plates do not verify the Saint Venant's principle anywhere. In that case the solution of the three dimensional model is mandatory even if its computational complexity could be out of the nowadays calculation capabilities.

The Saint Venant's principle was extensively used in the Ladeveze's works for defining elegant and efficient 3D simplified models [9]. This technique was then generalized to dynamics [11].

In the case of elastic behaviors the derivation of such 2D plate theory models is quite simple and it constitutes the foundations of classical plate and shell theories. Today, most commercial codes for structural mechanics applications propose different type of plate and shell finite elements, even in the case of multilayered composites plates or shells. However, in composites manufacturing processes the physics encountered in such multilayered plate or shell domains is much richer, because it usually involves chemical reactions, crystallization and strongly coupled and non-linear thermomechanical behaviors [1]. The complexity of the involved physics makes impossible the introduction of pertinent hypotheses for reducing *a priori* the dimensionality of the model from 3D to 2D. In that case a fully 3D modeling is compulsory, and because the richness of the thickness description (many coupled physics and many plies with different physical states and directions of anisotropy) the approximation of the fields involved in the models needs thousands of nodes distributed along the thickness direction. Thus, fully 3D descriptions may involve millions of degrees of freedom that should be solved many times because the history dependent thermomechanical behavior. Moreover, when we are considering optimization or inverse identification, many direct problems have to be solved in order to reach the minimum of a certain cost function.

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Today, the solution of such fully 3D models remains intractable despite the impressive progresses reached in mechanical modeling, numerical analysis, discretization techniques and computer science during the last decade. New numerical techniques are needed for approaching such complex scenarios, able to proceed to the solution of fully 3D multiphysics models in geometrically complex parts (e.g. a whole aircraft). The well established mesh-based discretization techniques fail because the excessive number of degrees of freedom involved in the fully 3D discretizations where very fine meshes are required in the thickness direction (despite its reduced dimension) and also in the in-plane directions to avoid too distorted meshes.

Thus, 3D solutions seem mandatory in many cases, however such solutions are not obvious because the numerical complexity that mesh based discretizations imply. Thus, new approaches able to address the efficient solutions of such models is required. In this manuscript we propose the application of the model reduction method known as Proper Generalized Decomposition – PGD – to the simulation of 3D thermomechanical models defined in plate geometries. This method is based on the use of separated representations. A space–time separated representation was originally proposed in the 80s by Pierre Ladeveze as one of the main ingredients of the LATIN (non-linear and non-incremental solver) and which was called "radial approximation" (the interested reader can refer to the Ladeveze works [10,12,13] the references therein). Then, this kind of separated representation was considered in the context of stochastic modeling by Nouy [16,17] as well as for addressing multidimensional models [2,3].

The separated representation basically consists in constructing by successive enrichment an approximation of the solution (defined in a space of dimension d) in the form of a finite sum of N functional products involving d functions of each coordinate. In contrast with the shape functions of classical discretization methods, these individual functions are unknown *a priori*. They are obtained by introducing the approximate separated representation into the weak formulation of the original problem and solving the resulting non-linear equations. If M nodes are used to discretize each coordinate, the total number of unknowns amounts to $N \times M \times d$ instead of the M^d degrees of freedom of classical mesh-based methods. Thus, the complexity of the method grows linearly with the dimension d of the space wherein the problem is defined, in vast contrast with the exponential growth of classical mesh-based techniques.

This strategy was successfully applied in our studies of the kinetic theory description of complex fluids. A multidimensional separated representation of the linear steady-state Fokker–Planck equation was introduced in the seminal work [2], further extended to transient simulations in [3] and non-linear Fokker–Planck equations in [14]. In [15,18], we considered the solution of Fokker–Planck equations in complex flows, where space, time and conformation coordinates coexist. We have also applied the same approach for solving the Schrödinger equation [5], the chemical master equation [6] or kinetic theory models formulated within the Brownian Configurations Fields framework [4]. For other applications the interested reader can refer to the review paper [7].

The fully three-dimensional solution of models defined in degenerate domains is also an appealing field of application of the PGD. Consider the unknown field $u(\mathbf{x},t)$ defined in a plate domain Ξ. Two approaches come to mind:

- Complete decomposition:

$$u(\mathbf{x},t) \approx \sum_{i=1}^{N} X_i(x) \cdot Y_i(y) \cdot Z_i(z) \cdot T_i(t). \tag{1}$$

This strategy is particularly suitable for separable domains, i.e. $\Xi = \Omega_x \times \Omega_y \times \Omega_z$. For general domains, embedding Ξ into a larger separable domain $\Omega_x \times \Omega_y \times \Omega_z$ can also be done, as described in [8].

- Plate-type decomposition:

$$u(\mathbf{x},t) \approx \sum_{i=1}^{N} X_i(x,y) \cdot Z_i(z) \cdot T_i(t). \tag{2}$$

This strategy is particularly suited when $\Xi = \Omega \times \mathcal{I}$, with $\Omega \subset \mathcal{R}^2$ and $\mathcal{I} \subset \mathcal{R}$. More complex domains (e.g. plates with a varying thickness) can be treated using an appropriate change of variable.
Because such decomposition involves the calculation of 2D functions $X_i(x,y)$ and 1D functions $Z_i(z)$ (these ones with a computational complexity negligible with respect to the computation of the 2D functions) we can conclude that the computational complexity of the fully 3D solution is of the same order of magnitude than the solution of 2D models, justifying the manuscript title.

We would like to emphasize that this paper does not concern a new plate theory proposal. This paper concerns the proposal of a new solution procedure able to compute efficiently fully 3D solutions of any model defined in plate domains whose numerical complexity reduces to the one characteristic of 2D solvers. It is important to notice that the results computed by applying the in-plane–out-of-plane separated representation can be only compared with the ones coming from standard 3D solutions, but not with the ones computed using classical plate or shell theories whose accuracy depends on the validity of the hypotheses introduced during the derivation of such simplified theories. The accuracy of our strategy must be evaluated by comparing the computed solution with the reference one, that could be obtained for example by using an accurate enough 3D finite element solution. The comparison of the solution computed by using our strategy and the ones obtained using different plate theories has no sense because we cannot consider these solutions as reference solutions (they are subjected to many hypotheses that fail, as argued above, in many cases). Solutions obtained by using a plate theory should be compared with fully 3D solutions to conclude on its accuracy, but in this work we are not concerned by such comparisons. In summary, we are not elaborating an alternative plate theory, but simply proposing a new algorithm for computing fully 3D solutions in degenerated plate domains, with a computational complexity characteristic of 2D solvers.

Undoubtedly, the connections between the PGD and different plate theories should be explored deeply. As we show later, in some circumstances, the first mode of the PGD solution has important resemblances with the solution obtained by applying standard plate theories, Mindlin or Kirchhoff depending on the plate thickness. Additional modes come to represent 3D effects that a simplified modeling (simple plate theories) is not able to capture. A deep analysis of all the connections existing between the PGD modes and standard and advanced plate theories constitutes a work in progress. This analysis could inspire new hypothesis to be introduced in advanced plate theories. Another interest of such a connection is defining bridges between plate models and fully 3D PGD descriptions to capture locally 3D effects in multidomain decompositions or multiscale frameworks. The first preliminary results of this study are extremely promising.

In the next section, the PGD is applied to perform an in-plane–out-of-plane separated representation for the steady state heat equation defined in a multilayered plate. The strategy is then generalized to elastic behaviors in Section 3. The accuracy and the numerical efficiency of the method are analyzed showing its full potential for the treatment of more complex composite structures. Finally, a parametric modeling case is addressed, in which the orientation of the different laminate plies is considered as extra-coordinates. As soon as the parametric solution is computed, only once and off-line, it can be particularized on-line for different values of the plies orientation on light computing platforms, as for example