ADVANCED MODEL ORDER REDUCTION FOR SIMULATING COMPOSITES FORMING PROCESSES

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Keywords: Composites forming processes, Numerical simulation, Model Order Reduction, Proper Generalized Decomposition, Real time simulation

Abstract

Efficient simulation of composites manufacturing processes remains today a challenging issue despite the impressive progresses reached in mechanical modeling, numerical analysis, discretization techniques and computer science during the last decade. Composites manufacturing involve multiscale models in space and time, highly non-linear and anisotropic behaviors, strongly coupled multiphysics and complex geometries. Moreover, optimization (shape and process optimization), inverse analysis (parameter identification, non destructive testing, ...) or process control need the solution of many direct problems, as fast and accurately as possible. In this context, model reduction techniques constitute an appealing simulation choice, making possible speeding-up computations of several orders of magnitude, and even, the solution of models never until now solved. In this framework real-time decision-making can be envisaged to allow process simulation to be used on the shop floor manufacturing, with the consequent impact in industrial practice. In this paper we combine several different modeling and simulation strategies for the efficient solution of a generic multi-physics and coupled problem. PGD allows defining offline the parametric pressure field related to the consolidation model, that is coupled with POD and RB based model order reduction that proceed online for solving the thermo-kinetic nonlinear model. The integration of all these models constitutes a *Simulation App* that allows real-time evaluation of any process conditions.

1. Introduction

Efficient simulation of composite manufacturing processes remains even nowadays, in many cases, a challenging issue, mainly when they involves rich 3D behaviors, multi-physics and the necessity of solving many scenarios very fast for optimization purposes. Below we revisit these issues and propose alternatives for alleviating all them within an efficient *Simulation App*.

Composites manufacturing processes involve many different physics. For instance, impregnation of fibrous reinforcements needs the efficient solution of models of flow through porous media that can be deformed due to the high momentum carried by viscous resin or the mould closing. Several issues

arise for such flows: their three-dimensional nature in several anisotropic and heterogeous fabrics with different orientations, the prediction of the permeability for each layer but also for the fibrous preform, the modeling of impregnation and prediction of residual porosity, among many others. A further aspect concerns the curing kinetics and its thermomechanical couplings in the case of thermosets.

Residual stresses are the main manifestation of all these physics and its prediction is a key point in order to optimize and/or control processes in order to limit the magnitude of the residual stresses induced deformations. All these coupled physics coexist and exhibit multiscale and localized behaviors in space and time. Due to the multiscale description, micro-macro modeling is mandatory, and appropriate interscale bridges, other than classical homogenization, must be defined.

Another important issue concerns the nature of the macroscopic models defined in plate or shell domains characterized by having a dimension (the thickness) several orders of magnitude lower that the other representative in-plane dimensions. This fact, even if it is not a major conceptual issue, is a real nightmare for simulation purposes. This situation is not new, plate and shell theories were successfully developed many years ago and they were intensively used in structural mechanics. These theories make use of some kinematic and static hypotheses to reduce the 3D nature of mechanical models to 2D reduced models defined in the shell or plate middle surface. In the case of elastic behaviors the derivation of such reduced 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 more complex, because as previously mentioned it involves chemical reactions, crystallization and strongly coupled thermomechanical behaviors. The complexity of the involved physics makes impossible the introduction of pertinent hypotheses for reducing the dimensionality of the model from 3D to 2D. In that case a fully 3D modeling is compulsory, and because of the need for a very detailed description in the thickness direction (many coupled physics and many plies differently oriented) the approximation of the fields involved in the models needs thousands of nodes distributed along the thickness direction. The well experienced mesh-based discretizations 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. The only solution to overcome that stalemate is to explore new discrezation 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, as well as the complex plates and shells assemblies usually encountered in composite structures.

Another important issue encountered in the simulation of composites manufacturing is the one related to the process control and optimization. In general, optimization implies the definition of a cost function and the search of the optimum process parameters defining the minimum of that cost function. The procedure starts by a guessed set of process parameters. Then the process is simulated by discretizing it. The solution of the model is the most expensive step of the optimization procedure. As soon as the solution is available, the cost function can be evaluated and its optimality checked. If the chosen parameters do not define a minimum (at least local) of the cost function, the process parameters should be updated and the solution recomputed. The procedure continues until reaching the minimum of the cost function. The solution of the process model is a tricky task that demands important computational resources and usually implies extremely large computing times. Thus, usual optimization procedures are inapplicable under the real-time constraint. The same issues are encountered when dealing with inverse analysis in which material or process parameters are expected to be identified from numerical simulation, by looking for the unknown parameters so that computed fields match the ones measured experimentally.

Until now the solution consisted in using the more and more powerful computing platforms and techniques for speeding up standard discretization techniques. Appealing alternatives for circumventing, or at least alleviating, these issues lies in the use of model reduction strategies. Model reduction is based on the fact that the solution of many models contains much less information that the one a priori assumed when the discrete model was built. Proper Orthogonal Decomposition, Proper Generalized Decomposition and Reduced Basis are nowadays widely considered from a fundamental and applicative viewpoints.

Proper Orthogonal Decomposition (POD) is a general technique for extracting the most significant characteristics of a system's behavior and representing them in a set of "POD basis vectors." These basis vectors then provide an efficient (typically low-dimensional) representation of the key system behavior, which proves useful in a variety of ways. The most common use is to project the system governing equations onto the reduced-order subspace defined by the POD basis vectors. This yields an explicit POD reduced model that can be solved in place of the original system. The POD basis can also provide a low-dimensional description in which to perform parametric interpolation, infill missing or "gappy" data, and perform model adaptation. There is an extensive literature on POD showing it has broad application across fields. Some review of POD and its applications can be found in [3, 12, 19, 20] and the references therein.

Another family of model reduction techniques lies in the use of Reduced Basis constructed by combining a greedy algorithm and "a posteriori" error indicators. As for the POD, the Reduced Basis method requires some amount offline work, but then the reduced basis model can be used online for solving different models with control of the solution accuracy, because the availability of error bounds. When the error is unacceptably high, the reduced basis can be enriched by invoking a greedy adaption strategy. Useful review works on the subject are [13, 15, 17, 18].

Techniques based on the use of separated representations are at the heart of the so-called Proper Generalized Decomposition (PGD) methods. Such separated representations were first considered in the Hartree-Fock and post-Hartree-Fock methods. Then, they were used for separating space and time in transient solutions [14]. Separated representations were employed for solving multidimensional models suffering the so-called curse of dimensionality [1, 2] and in the context of stochastic modeling [16]. Then, they were extended for separating space coordinates making possible the solution of models defined in degenerated domains, e.g. plate and shells [4, 5] as well as for addressing parametric models where model parameters were considered as model extra-coordinates, making possible the offline calculation of the parametric solution that can be viewed as a metamodel or a computational vademecum, to be used online for real time simulation, optimization, inverse analysis and simulation-based control [9]. Some recent reviews concerning the PGD can be found in [6–8] as well as in the recently published primer [11].

This work is intended to illustrate the potential of considering model order reduction techniques to enhance adaptability of composite manufacturing process to changeable material and process environments through increased parametric modeling capabilities. The process selected is the consolidation and curing of a real part. Consolidation and curing of thermoset prepregs involve different physics: heat transfer, compression of fiber beds, resin flow and chemical reaction. Strong couplings exist between these physics and many material parameters come into play. In this paper we combine several different modeling and simulation strategies for the efficient solution of a generic multi-physic and coupled problem. The integration of all these models constitutes a *Simulation App* that allows real-time evaluation of any process conditions. The described methodology can be extended and generalized to other processing technologies.



Figure 1. Analyzed part (left) and problem geometry (right).

2. Composite OGV manufacturing: Curing and consolidation modelling

We consider the composite OGV shown in Fig. 1 (left), manufactured by press forming and curing of thermoset unidrectional continuous fiber prepregs. During the forming process the composite lay-up is heated by conduction from the metallic mold walls and consolidated under press. The heat initiates the cure reaction and the applied pressure provides the force needed to drain the excess resin out of the composite, consolidate prepreg layers and reduce voids by compressing the air inside. Because of the heating process the thermoset resin starts its cure, that implies: (i) the thermal coupling because the curing exothermic effects; (ii) the change of thermal and kinetic parameters because their thermal dependence and also because most of them depend on molecular crosslinking; and (iii) the rheology modification because the resin viscosity depends on the degree of cure.

The thermo-kinetic model is given by the energy balance equation

$$\rho \frac{\partial}{\partial t} (C_p(T, \alpha)T) = \lambda \nabla^2 T + \rho \Delta H \dot{\alpha}, \tag{1}$$

where without loss of generality, it was assumed that the resin density ρ remains almost constant and the thermal conductivity of the composite λ is considered constant within the process window. These assumptions follow the kinetic characterization of the employed resins. Heat convection is neglected because of the creeping flow approximation and it is assumed there is no dispersion effect, i.e. resin and fiber share the same temperature. In the previous expression $T(\mathbf{x}, t)$ represents the temperature field, C_p the specific heat of the composite that depends on the temperature and the degree of cure α and ΔH is the enthalpy related to the curing reaction.

The energy balance equation must be complemented with the kinetic equation describing the curing reaction advancement, that is formulated in the most general form from the non-linear evolution equation

$$\dot{\alpha} = f(T, \alpha). \tag{2}$$

The solution of the thermo-kinetic model requires defining appropriate initial and boundary conditions. The initial conditions are given by $T(\mathbf{x}, t = 0) = T_0$ and $\alpha(\mathbf{x}, t = 0) = \alpha_0$. It is important to note that the heat conduction equation (1) is global in space whereas the kinetic equation (2) is local, that is, it applies and must be solved at each position from the temperature history existing at that position.

Boundary conditions are only needed for the heat conduction equation, and in particular they concerns the prescribed temperature evolution at the top and bottom surfaces S^+ and S^- (see Fig. 1, right), that read respectively $T(\mathbf{x} \in S^+, t) = T_t(t)$ and $T(\mathbf{x} \in S^-, t) = T_b(t)$. When the prescribed temperatures do not evolve in time, they reduce to constant values, T_t and T_b respectively. The heat losses through the lateral surfaces \mathcal{L} (see Fig. 1, right) can be neglected, that results in $\nabla T(\mathbf{x}, t) \cdot \mathbf{n} = 0$, being **n** the unit outwards vector defined on \mathcal{L} .

In general, process optimization could involve the adequate choice of these four process parameters: T_0 , α_0 , T_t and T_b .

The consolidation drains the excess resin out of the composite. Assuming that only the resin moves between fibers, that is, preform is compressed but remains nearly stationary, the resin flow model can be described from the Darcy's flow model:

$$\begin{cases} \nabla \cdot \mathbf{v}(\mathbf{x}) = 0\\ \mathbf{v}(\mathbf{x}) = -\frac{\mathbf{K}(t)}{\eta(T,\alpha)} \nabla P(\mathbf{x}) \end{cases}, \tag{3}$$

where it is emphasized the fact that the permeability **K** evolves in time because the part is compressed with a given compression rate \dot{U} . On the other hand because the curing reaction advances the resin viscosity η will tend to increase until the flow is no longer possible or will induce fiber washing.

The solution of the flow model also requires adequate boundary conditions. In particular it is assumed that in the lateral boundaries \mathcal{L} (see Fig. 1, right) pressure vanishes, that velocity at the top surface corresponds to the compression rate \dot{U} assumed directed in the vertical direction and that the resin velocity vanishes at the bottom surface, that is:

$$\begin{cases} P(\mathbf{x} \in \mathcal{L}) = 0\\ \mathbf{v}(\mathbf{x} \in \mathcal{S}^+) = (0, 0, -\dot{U})^T \\ \mathbf{v}(\mathbf{x} \in \mathcal{S}^-) = \mathbf{0} \end{cases}$$
(4)

3. Simulation App

The *Simulation App* for the OGV manufacturing process is a process-specific application that allows the user to simulate almost in real time different process conditions and visualize the simulation results. The user interacts with the *Simulation App* through a basic Graphics User Interface (GUI). In order to demonstrate the feasibility and potentiality of this kind of applications, we developed a demonstration version of the *OGVApp* in the MATLAB environment using GUIDE. This allows creating the GUI very easily. The MATLAB Application Compiler was used in order to create a standalone version of the code that could be easily transferred to the final user for demonstration purposes. Other proper implementations are of course possible although not explored in this paper, as they are outside of its scope.

The concept of a Simulation Application offers several potentialities. Since the application is processspecific, rather than implementing a general purpose visualisation environment, it is possible to first identify the set of outputs of interest and then implement a simple and specific visualization interface. For example, if we know in advance that the maximum pressure gradient is an important indicator for defects, as it is the case in OGV manufacturing processes, we can include a functionality that displays the maximum pressure gradient and its location, at each time step. Then, the user can access to this information by simply activating a checkbox.

A similar discussion can be addressed regarding the data input. A general purpose simulation code needs to be fed with simulation parameters, which possess a physical meaning in the mathematical model to be solved. In order to get to these, the user must convert process parameters (measures, for instance) into simulation parameters before running the simulation. A Simulation Application, since it is process-specific, can perform this conversion automatically according to rules provided. Therefore, the user

only enters process parameters, which are natural to them, into the application. The difference between process and simulation parameters is kept almost transparent to the user in the GUI. In consequence, a Simulation Application is not only simulation tool but it also integrates the process knowledge via process-specific inputs and outputs.

The OGVApp is composed of three modules:

- 1. *Pre-processing.* This module performs two basic operations: data loading and parameters conversion. Data loading simply reads all pre-computed data required to run the reduced model. This operation only needs to be done once after launching the application, and it is performed in the GUI via the Load Data button. Parameters conversion gathers data entered by the user and computes the simulation parameters. This operation is performed in the GUI via two different tabs: the Parameters Tab, in which some default values that normally do not change are proposed (e.g. resin and fiber specific weight), and the Data Tab, in which process parameters are defined (e.g. temperature cycle, closure rate, etc.). The conversion operation is launched by the Update button, and the initial degree of curing and the initial fiber volume content, both being simulation parameters, are computed.
- 2. *Simulation*. This module is driven by a principal function that governs the interaction between the two reduced models explained in previous sections: POD reduced model for the thermo-kinetics simulation and PGD reduced model for the consolidation (Darcy's equation) simulation. Basically, this module takes all data defined in the pre-processing module and runs the POD model in the time interval of interest defined by the user. The user can also choose the number of equally spaced time frames at which the solution wants to be accessed. The pressure field can be then obtained at each time step by evaluating the PGD parametric solution using the POD-based thermo-kinetic solution at the corresponding times.
- 3. *Visualization*. A process specific visualization module has been implemented in the OGVApp. The reduced model produces seven scalar fields: curing degree, temperature, viscosity, pressure and the three components of the pressure gradient. They are displayed simultaneously on the external boundary of the part as well as in five sections (see Fig. 2). The section view is necessary to appreciate, for instance, the temperature evolution inside the part. Several quantities of interest, such as the maximum and minimum pressure gradient as well as their location, can be also displayed.

Model reduction based simulation App can be a powerful tool for complex composite processes to increase the entitlement yield by adapting for the variation that comes from material chemistry and physical properties in addition to thermal and pressure histories applied during the process. Typical entitlement yield is limited because of the inherent variations and multi-physics interactions. Part quality loss is due to either (i) internal defects, (ii) not meeting dimensional requirements or (iii) poor internal fiber matrix structure. A successful manufacturing process must minimize all three quality components. Simulation App can be implemented in the manufacturing process seamlessly to make real-time decisions regarding process adaptation possible overcoming inherent variation and truly increasing the entitlement yield of the process. As an example, the OGVApp will take real process measurements as inputs which capture the incoming variation in the pre-processing section and provide quantities of interest e.g. maximum pressure gradient that can be relate to quality. If the quality does not meet requirements, pre-computed sensitivity results can be used to identify corrective process change to bring it within requirements. The corrective process change can be as simple as choosing among predefined process cycles. All this can be made possible only because of real-time models capable of reflecting physics of the entire process.



Figure 2. OGVApp visualization: temperature field at t = 0 (top) and pressure field at t = 1.05 min (centre).

4. Conclusions

In this work we investigated the use of different model order reduction techniques for addressing a multiphysics model involved in composite OGV manufacturing processes. The strategy we proposed is based on the calculation of the parametric solution of the 3D flow model that is coupled with the solution of the thermo-kinetic model. The last one, can be easily solved online using an adequate reduced basis. Thus, in the online stage the online thermo-kinetic solver dialogue with the flow parametric solution, allowing spectacular computing time savings. All the numerical tools were integrated in a *Simulation App* able to compute in real time the process response for any choice of the process parameters.

Even if the methodology has been discussed on a practical case-study, of real industrial interest, it can easily generalized for considering different process models. Although methodology has been discussed in context of real industrial application, it could be applied to different physical models and processes. However, possibility of having models capable of providing results in real-time (less that 10 sec) creates a new paradigm for complex manufacturing processes going from reactive to adaptive manufacturing.

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