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Computational Environment for the Multiscale, Multi-Physics Resin Transfer Molding Process

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Summary

The capability to predict the residual stresses induced during the manufacturing process in composite components is necessary for the timely fielding of new combat systems. At the U.S. Army Research Laboratory we have developed a computational environment to model the resin flow, heat transfer, curing, and residual stresses in composite components manufactured with the resin transfer molding (RTM) process. This computational environment uses object-oriented programming methods to provide model coupling capabilities and access to high performance computing assets. In this paper we will provide details of the physical models, software, and the validation/verification procedure used to develop this RTM simulation package.

Introduction

The resin transfer molding (RTM) process is used extensively to produce light weight composite structures at a low cost. The simulation of the RTM process requires multi-physics simulations that predict the resin flow through a porous media and the heat transfer from resin to fiber and surrounding mold. An accurate RTM model must also consider the exothermic resin curing process. After the resin has cured, residual stresses develop in the composite part during cool down to room temperature. Analysis of these residual stresses requires a multiscale approach that considers the fiber-resin microstructure.

In order to assist in the timely coupling and parallelization of the computational models required for this analysis we developed the Simple Parallel Object-Oriented Computing Environment for the Finite Element Method (SPOOCEFEM) [1,2]. SPOOCEFEM is a general purpose finite element method (FEM) framework for developing multi-physics/multiscale applications for use with parallel computer architectures.

RTM Finite Element Model

The flow of the resin through the fibrous preform is modeled using Darcy's Law for flow through a porous media. A detailed description of the implicit algorithm based on the pure FEM can be found in Mohan et al. [3] and Ngo et al. [4]. The semi-discrete equation used to solve the resin flow analysis problem is given in

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equation 1

$$C\dot{\Psi}+KP=q \tag{1}$$

where C is the lumped mass matrix, $\dot{\Psi}$ is the nodal fill rate, K is the permeability matrix, P is the nodal pressure results, and q is the resin mass flow rate at the mold boundary.

Heat transfer in the RTM manufacturing process is modeling using the integral form of the mass balance equation [5]. The thermal model equations employ an energy balance equation based on a fiber-resin thermal equilibrium model [6], and after discretization can be written in the form of equation 2.

$$C\dot{T}+(K_{ad}+K_{cond})T=Q_q+Q_{\dot{G}} \tag{2}$$

In equation 2, $\dot{T}$ is the rate of temperature change, K_{ad} and K_{cond} are the advection and conduction matrices, respectively. T is the nodal temperature distribution, and Q_q and $Q_{\dot{G}}$ are the boundary thermal flow rate and volumetric heat generation terms, respectively.

The degree of resin cure, α, and associated heat generation is tracked by solving equation 3.

$$C\dot{\alpha}+K\alpha=Q_{R_\alpha} \tag{3}$$

In equation 3,$\dot{\alpha}$ is the rate of cure and Q_{R_α} is the rate of the curing reaction.

By coupling the resin cure and heat transfer models with the resin flow model through sub time stepping it is possible to accurately describe the mold filling process. By assuming that until the resin has cured no residual stresses form in the composite part we can decouple the filling simulation from the residual stress calculation.

The residual stress computation requires knowledge of the microstructure of the composite material in order to accurately predict the mechanical properties of the composite part. The Asymptotic Expansion Homogenization (AEH) method [7] is used to homogenize the properties of the heterogeneous composite microstructure. The actual implementation used in this effort is based on the work of Chung [7].

Software Development

The SPOOCEFEM framework was developed at the U.S. Army Research Laboratory (ARL) in order to speed the development of multi-physics FEM applications and to easily port them to parallel computers. The details of SPOOCEFEM are reported elsewhere [1,2] but some of the features that simplify model coupling will be repeated here. There are two types of model coupling possible with SPOOCEFEM. The first method is tight coupling, where class inheritance is used to access the data and routines of an existing model. The second method is loose coupling, where a standard data file format, namely the eXtensible Data Model and Format (XDMF) [8], is used to pass data between models.

SPOOCEFEM is built upon many open source libraries that are used to provide the required functionality for FEM applications. This building block approach is illustrated in figure 1. In figure 1 the HDF5 and Expat libraries are used by the XDMF for data storage and description. VTK provides visualization of scientific data capabilities and PETSc and PSPASES contain linear equation solvers required by most FEM applications.

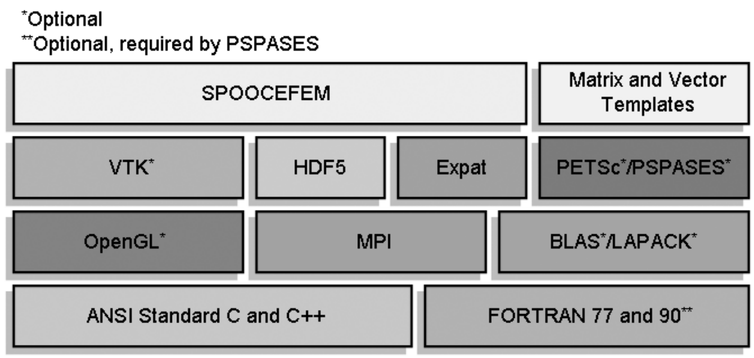

Figure 1: Building block diagram of SPOOCEFEM framework.

We have used the SPOOCEFEM framework to couple the resin flow, heat transfer, and resin cure kinetics models together. SPOOCEFEM uses inheritance of classes in order to utilize existing models and tightly binds them together to form a single multi-physics application. By using multiple inheritance it is possible to quickly add the thermal and cure kinetics models to the already implemented resin flow model while taking advantage of any future enhancements to the resin flow model. For example, in figure 2 the PhoenixFlowElement2dTri3 class that contains the routines for a 3-noded triangular element used to model heat transfer in the RTM process inherits the flow model routines from the ComposeElement2dTri3 class.

Since the residual stresses are assumed to form only after the resin has cured, and that occurs after the mold has completely filled we have chosen to loosely couple the thermal and residual stress models. This is done by storing data in the XDMF format that is used by all applications developed with SPOOCEFEM. XDMF I/O can also be easily added to existing applications negating the need for redevelopment in the SPOOCEFEM framework. The residual stress model itself is a multiscale model and these scales are tightly coupled using SPOOCEFEM. An example of a micro-scale model for a woven fabric is shown in figure 3, along with the corresponding macro-scale model.

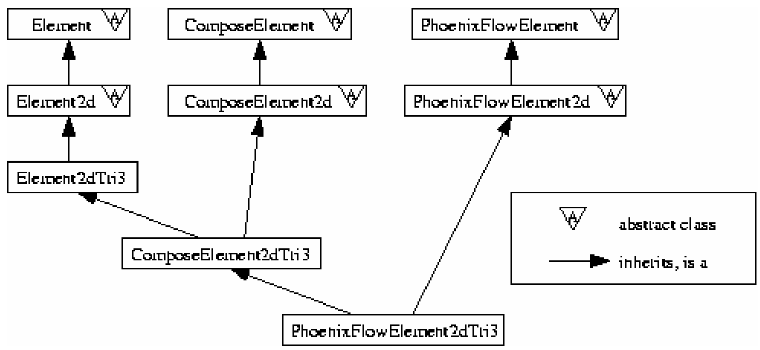

Figure 2: Hierarchy of the 3-noded 2-D element class that inherits the resin flow model capabilities from the ComposeElement2dTri3 class.

(a) (b)

Figure 3: Multiscale model used in residual stress computations. a) Micro-scale unit cell model of woven fabric and resin. b) Snapshot of macro-scale composite part model.

RTM Software Enhancements

In addition to the ability to model the heat transfer and compute the residual stresses in the RTM process we have included many enhancements. One of the more useful is the addition of the "one-shot" [9] filling algorithm. In this algorithm the resin viscosity is assumed to be constant and the last point in the mold to fill and the time to fill the mold are computed by solving two linear equations. This typically provides a good estimate of the mold fill time prior to simulating the process with heat transfer considered. The second enhancement is the addition of automated optimization [10] and sensitivity analysis [11,12]. By combining these methods it is possible to optimize the RTM process parameters by considering any derived cost function of interest to the process engineer.

Software Validation and Verification

During the development of this software package extensive verification and validation (V&V) was carried out. Because the developments here involved parallel computations the results from various numbers of CPUs up to 512 where checked to verify that the simulation results were correct to machine accuracy. The resin flow and thermal results were validated against analytical models when available also for simple geometries and against published experimental results. An external review of the V&V was carried out for the beta test of the developed software with positive results.

Conclusions

Using SPOOCEFEM and XDMF we have successfully coupled mutli-physics/-multiscale models in order to accurately simulate a complex manufacturing process, namely the RTM process. In addition, SPOOCEFEM provides parallel processing capabilities, allowing for the modeling of much larger components, with little effort by the application developer. The residual stress data produced from these models provides the basis for an accurate consideration of the mechanical and impact modeling of as-manufactured composite parts. This is invaluable in the rapid development, prototyping, and deployment of new composite-based systems.

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