Voxel Based Stochastic Modeling of Complex Materials

Manuel Ignacio Balaguera[*1], Jenny Paola Lis[#2], Mercedes Gaitán[#3], Amelec Viloria[+4], Paula VivanaRobayo Acuña[#5], Henrry LaVerde[#6]

[*]School of Mathematics and Engineering, FundaciónUniversitaria Konrad Lorenz, Bogota, Colombia
[#]School of Business, FundaciónUniversitaria Konrad Lorenz, Bogota, Colombia

[+]Universidad de la Costa, Barranquilla, Colombia

Abstract

In the present paper an object oriented stochastic approach is proposed for the construction of synthetic, computational models of complex materials. The conventional approach to model and study materials mechanics will be outlined, indicating its limitations to deal with complex heterogeneous materials. The proposed object oriented integrative modeling will be explained emphasizing its advantages compared to continuum mechanics when dealing with complex materials. Finally, the stochastic assembly of complex materials synthetic samples is described and the architecture of the 3M2S (Multiphysics Materials Modeling and Simulation System) is shown, indicating further work based on 3M2S.

1. Introduction

The limited availability of natural resources and the high diversity of specific properties and behaviors imposed to the materials used in high tech industry and health, has motivated an increased interest in the design and development of smart materials: materials with a high adaptability capable to respond in a controlled fashion to changes in the physicochemical environment and to external signals.

Those smart materials(1)are complex systems(2), since they are composed by a high diversity of objects, some of them with a certain degree of autonomy (cells, nanodevices, nanoparticles). In addition, those materials are highly heterogeneous and anisotropic in their physical (mechanical, thermal, electromagnetic, optical) and chemical properties(3).

As a result, existing mathematical models for those physical properties and behaviors cannot represent such a complexity in order to explore the tightly coupled phenomena occurring as a consequence of changes and interactions produced by objects and systems (sometime biological)scattered across a multiplicity of organization levels present incomplex adaptive systemssuch as biological tissues or artificial smart materials(4).

In the present paper, an object oriented stochastic approach(5)is proposed for the construction of synthetic, computational models of complex materials. By using object oriented methods(6) it is possible to create a digital sample of a complex material that allow to keep record of the individual states and dynamics for each component, in this case a voxel(7). In addition, thanks to object oriented methods it is possible to define autonomous components (cellular automata) which contains individually a set of "programs" (methods) allowing their adaptation to the surrounding environment and to respond to external signals. The assembling of a macroscopic sample of the complex material is made by a stochastic process choosing at random from a base set of different structure voxels chosen in agreement with probability distributions built from data obtained using real materials samples.

In the present paper the basic principles and components of the proposed methodology will be explained and in a next publication, the results of validated simulations experiments will be accounted.

2. Review of the analytical approaches, their background and limitations(8)

Despite the unlimited diversity of materials, physics classifies them in a small set of abstract categories: particles, rigid solids, deformable solids, fluids, viscoelastic bodies and some additional specialized categories.

Actually, this is an artificial classification because depending upon the spatial and temporary scales of observation and on the range of applied forces, any body may be classified in any category.

When a given set of forces or a force field is applied to an elastic body, there is a "volumetric distribution of force" in the body which is characterized by a stress field and a strain field. Those fields together represent the complete mechanical state of the body.

From a general perspective, stress and strain in a body point and in its neighborhood are mathematically represented by tensor mathematical objects. Generally speaking, a tensor is a 3x3 matrix used to quantify an anisotropic physical quantity, where each row corresponds to a vector representing the projection of the tensor along the normal to a symmetry plane of the body.

In order to illustrate visually what tensors are and how to represent them, let us consider what occurs with a hollow cylinder with a thick wall.

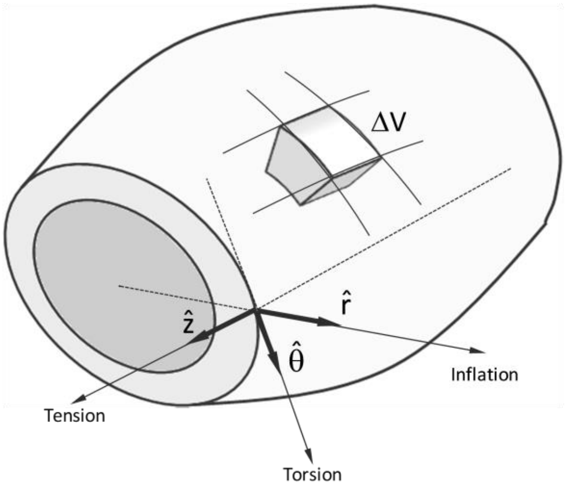

Figure 2.1 Axis for stress tensor in a hollow cylinder with a thick wall

As shown in figure 2.1, the cylinder has three symmetry directions: radial, circular and axial. Each direction corresponds to one point cylindrical coordinate: r, θ and z, respectively and to a deformation mode: volumetric (inflation): change in "r", torsion: change in "θ" and tension (traction, axial) change in "z".

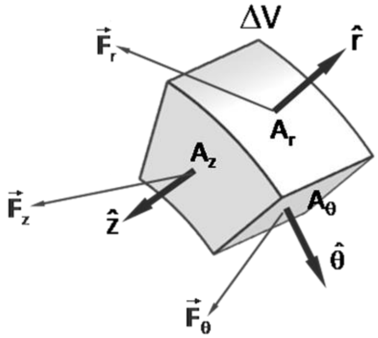

Figure 2.2 Stress tensor components

As illustrated by figure 2.2, the stress tensor is the matrix composition of three stress vectors, each one corresponding to a plane of symmetry:

$$\vec{\sigma}_r = \sigma_{rr}\hat{r} + \tau_{r\theta}\hat{\theta} + \tau_{rz}\hat{z} \text{where } \sigma_{rr} = \frac{1}{A_r}\vec{F}_r \cdot \hat{r},\ \tau_{r\theta} = \frac{1}{A_r}\vec{F}_r \cdot \hat{\theta},\ \tau_{rz} = \frac{1}{A_r}\vec{F}_r \cdot \hat{z} \qquad \text{(2.1.a)}$$

$$\vec{\sigma}_\theta = \tau_{\theta r}\hat{r} + \sigma_{\theta\theta}\hat{\theta} + \tau_{\theta z}\hat{z} \text{where } \tau_{\theta r} = \frac{1}{A_\theta}\vec{F}_\theta \cdot \hat{r},\ \sigma_{\theta\theta} = \frac{1}{A_\theta}\vec{F}_\theta \cdot \hat{\theta},\ \tau_{\theta z} = \frac{1}{A_\theta}\vec{F}_\theta \cdot \hat{z} \qquad \text{(2.1.b)}$$

$$\vec{\sigma}_z = \tau_{zr}\hat{r} + \tau_{z\theta}\hat{\theta} + \sigma_{zz}\hat{z} \text{where } \tau_{zr} = \frac{1}{A_z}\vec{F}_z \cdot \hat{r},\ \tau_{z\theta} = \frac{1}{A_z}\vec{F}_z \cdot \hat{\theta},\ \sigma_{zz} = \frac{1}{A_z}\vec{F}_z \cdot \hat{z} \qquad \text{(2.1.c)}$$

Where σ_{ii} holds for normal stresses and the τ_{ij} elements are used to represent shear stress. Finally, the complete stress tensor is:

$$\sigma = \begin{bmatrix} \sigma_{rr} & \tau_{r\theta} & \tau_{rz} \\ \tau_{\theta r} & \sigma_{\theta\theta} & \tau_{\theta z} \\ \tau_{zr} & \tau_{z\theta} & \sigma_{zz} \end{bmatrix} \qquad \text{(2.2)}$$

In the conventional approach (continuum mechanics and its numerical extension, the finite element method) the mechanical behavior of materials is "governed" by Hooke's tensor law:

$$\sigma = E\ \varepsilon \qquad \text{(2.3)}$$

Where E is the Young's (elastic) modulus tensor for the material and is the strain tensor.

In continuum mechanics, the hardest case is for orthotropic[1] materials whose physical properties parameters have spatial change in agreement with rules expressed by tensor functions of position (tensor fields). That restrictions or work hypothesis fit very well for

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[1] An orthotropic material allows change in physical properties depending upon each of three orthogonal axis.

crystalline materials, even for glasses where the uniformity of randomness guarantees ergodicity[2] and, as a consequence, the use of statistical physics.

For a complex material sample, the fact that some of its components may be autonomous objects inhibit the possibility to express its states probabilities only as dependent upon its energy and, in this way there is breaking of ergodicity and as a consequence the inadequacy of statistical mechanics principles (mainly the principle of equipartition) in the development of models for such a complex material.In the next section the main aspects of object oriented integrative modeling of complex Systems will be explained and justified.

3. Object oriented integrative modeling of a complex material sample

Thanks to the main features of object orientation: classification, encapsulation, inheritance and polymorphism, it is possible to automaticallycreate and assemblea huge number of component objects coming from a diversity of classes whose definition may encapsulate specific and particular properties and sets of behavior rules.

In object oriented integrative modeling the starting point is the analysis of the system to be modeled beginning with a hierarchical decomposition into different levels of structural categories, represented by the concept of "class" in the object oriented approximation.

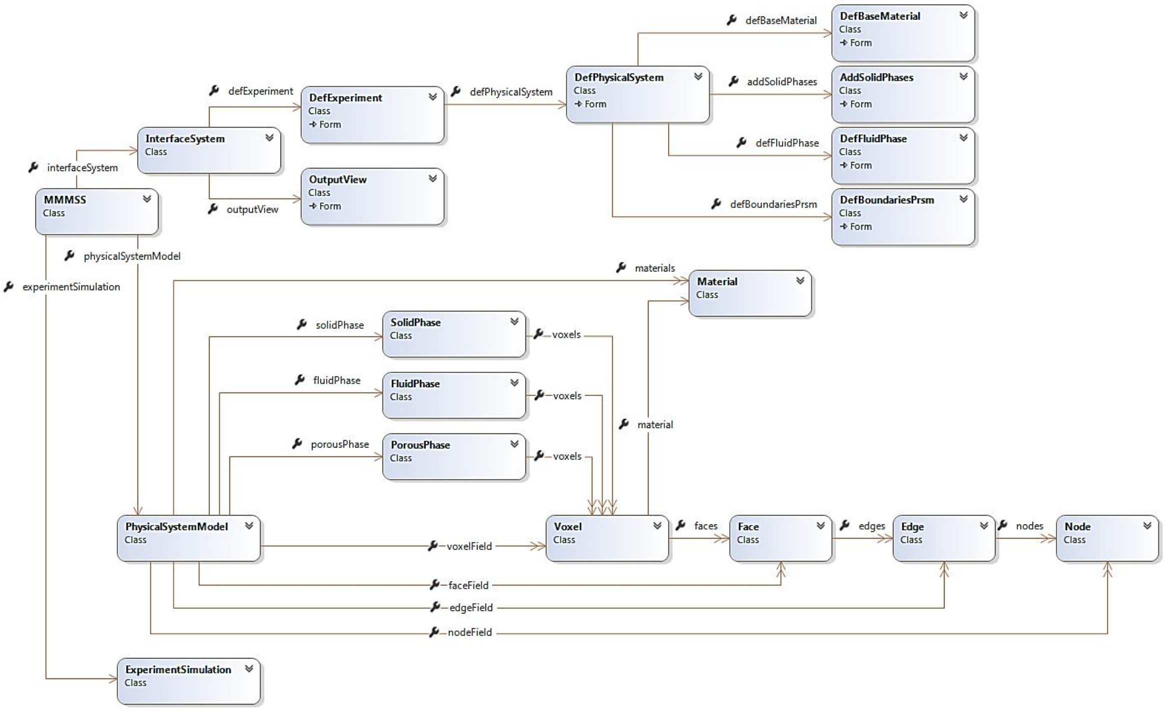

Figure 3.1.a

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[2] The probability associated with a given ergodic system state depends only of the system's energy (the value of its Hamiltonian function) and its averages on time coincide with averages over its possible configurations.

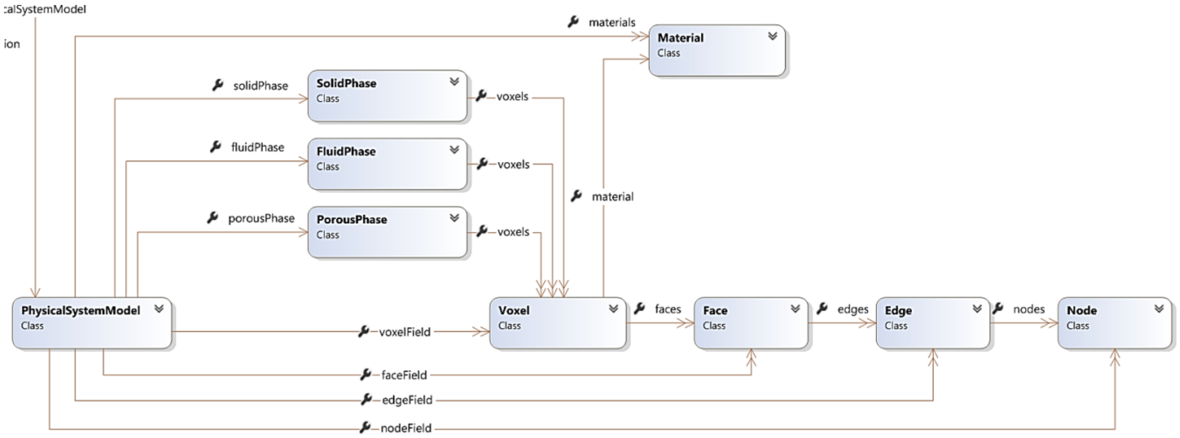

Figure 3.1.b

Both, figures 3.1.a and 3.1.b are UML (Unified Modeling Language) Class Diagrams(9). A class diagram displays the different categories of objects, classes, composing a complex system and its relations, in this case, composition relations:

In 3.1.a, the class diagram corresponds to the planned structure for 3M2S (Multiphysics Materials Modeling Simulation System), in development by the author, that will allow to realize simulation experiments about the multiphysics response (mechanical, thermal, fluid diffusion and chemical reactions) of a complex material.

In agreement with the 3.1.a class diagram, in order to create the class experiment, it will be necessary to create three composing objects, each one belonging to one of the three classes: physical system, simulation and interface.Notice that the double tipped arrows indicate an array of components.

The physical system will be the composition of a solid structure (porous), a fluid phase (liquid or gas) and a thermal field, defined at each point (node) of the solid structure and at each point of the fluid phase.

The simulation component of the experiment will be composed by a simulation scenario which defines the external agents acting on the material sample: arrays of mechanical loads, fluid and heat sources. In addition, the simulation class include as components all the boundary and initial conditions for the experiment.

The simulation class is also equipped with a set of mathematical engines necessary to process the time evolution of each component and the complete system: a Monte Carlo (Metropolis) engine used to simulate all stochastic processes involved in the experiment, a finite element method engine used to simulate the mechanical behavior of the solid phase and, if necessary, the heat diffusion. Depending upon the type of fluid phase, the behavior of each fluid phase will be simulated by using the most convenient fluid dynamics engine chosen between a Lattice Boltzmann engine and a Molecular Dynamics engine.

Finally, regarding the 3.1.a experiment class diagram, it is necessary to include a user interface composed byan input interface for information source specification and a simulation output interface which may be a set of 2D xy like plots or a 3D structure and fields visualizator.

The figure 3.1.b presents the class diagram representing the hierarchical structure of the material sample model which is visually represented in figure 3.2. In agreement with the diagram, the objects composing a material sample, from bottom level to top level belong to: 1. Node class, 2. Edge class, 3. Face class, 4. Voxel class and 5. Solid class. Those classes are hierarchically arranged as linked lists: an edge is an one dimensional object defined by a list of two nodes, a face is an array of edges forming a 2D polygonal region (generally quadrilateral or triangular), a voxel is a closed 3D region limited by e polyhedron, it is useful to use quadrilateral prisms or tetrahedrons, and, finally the solid is an array of voxels.

This hierarchical composition allows us: 1. To individually handle and keep record of the state of those diverse components in agreement with physical principles, 2. Associate different structure components with respective physical objects: the solid is a structure formed just by edges which gives account of the mechanical behavior of the solid, fluids and vacuums occupy and diffuse across voxels, and thermal fields are temperatures associated with each voxel. 3. Detect special events as face collisions and associate them with fracture. 4. Build up different field visualizations.

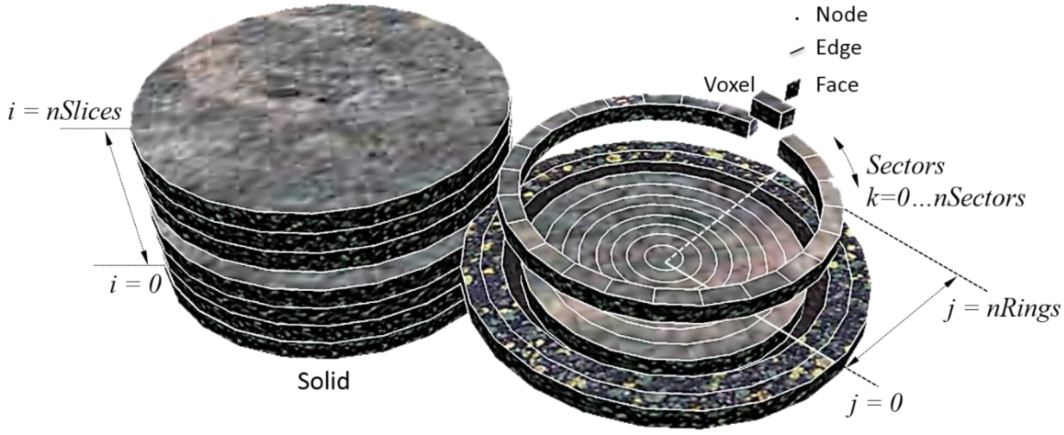

Figure 3.1 Hierarchical structure to voxelize a complex material sample

as an example, Figure 3.1 illustrates a hierarchical observational decomposition of a cylindrical sample used to implement a stochastic model allowing to keep track of the state and evolution of all components in each hierarchical level. As generally the experimental samples have a regular shape (a cylinder or a rectangular prism) the sample assembling process may be organized by hypothetic substructures: here, for easy navigability, the lists indexes are arranged as: "i" for slices, "j" for rings, "k" for (circular) sectors, as to allow the use the algorithm shown in code 1:

```
Input sample height and radius
    Define and calculate step size for slices
    for i=0 to nSlices
        Define and calculate step size for rings
        for j=0 to nRings
            Define and calculate step size for sectors
                for k=0 to nSectors
                    Create node list //*each node is an object
                Create edge list //* each edge is an object
```

```
            Create face list //* each face is an object
        Create voxel list //* each voxel is an object
```

Code 1: pseudocode algorithm for sample model assembly

In the creation of the different objects composing the model a stochastic association between mechanical, thermal, fluid and chemical properties withmodelobjects can be established: mechanical with edge object list, thermal, fluid and chemical with faces ad/or voxels.

4. Conclusions and Further work

1. In the present work, object oriented methods for modeling complex materials has been presented and compared with continuum mechanics, remarking its advantages.
2. The hierarchical decomposition of the material sample has been presented and explained by using class diagrams, which facilitates code implementation and maintenance as allow to keep individual record and control of each component object.
3. It has been presented an algorithm for the sample assembly in the case of regular solid samples, a cylinder here. This algorithm together with appropriate probability distributions for material phases and components and a dataset coming from real samples characterization will allow to reproduce the high space heterogeneity of a complex material.

   As a second phase of the project, the 3M2S (Multiphysics Material Modeling and Simulation System) will be implemented and validated by comparing simulation experiments results with corresponding experimental data.

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