Periodic three-dimensional mesh generation for particle reinforced composites with application to metal matrix composites

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A method for the generation of three-dimensional model microstructures resembling particle reinforced composites is developed based on the periodic Voronoi tessellation. The algorithm allows for the generation of arbitrary particle volume fractions and produces periodic geometries based on the erosion procedure suggested by Christoffersen (1983). A technique for the creation of high quality periodic spatial discretizations of the particle systems for application with the finite element method is described in detail. The developed procedure is extensively applied to metal ceramic composites (Al-ScC) at volume fractions ranging from 10 to 80%. The elastic and thermo-elastic material properties are investigated and the effect of higher statistical moments (see, e.g., Torquato, 2002), i.e. of the particle shape and relative position, is evaluated in terms of constraint point sets used in the generation of the random microstructures.

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1. Introduction

The effective properties of heterogeneous materials are much sought-after quantities. In order to computationally predict the effective behavior of heterogeneous materials it is necessary to first find a precise topological description of the considered microstructure. Unfortunately, the acquisition of this information is hindered by a multitude of problems. A popular experimental technique is the serial sectioning using either polishing (Ganesh and Chawla, 2005) or the FIB (focus ion beam) technique (Groebler et al., 2006) combined with optical or electrical measurements. Another is the X-ray micro computer tomography (e.g., Madhavan et al., 2007). All these methods share a considerable sensitivity with respect to certain physical properties, e.g., electrical conductivity or the local mass density of the material. This renders the choice of a suitable experimental method a challenging procedure. Further, many of the mentioned techniques are destructive, i.e. they do only allow for limited (if any) in situ measurements, or for verification of the computed results (at least in the non-linear regime). When statistical studies with respect to different microstructures are aspired, then the effort for experimental techniques can be achieved by recourse to the statistical properties of the microscopic medium. The latter are, generally, determined by the n-point statistics of the material (see, e.g., Ohser and Mücklich, 2000; Torquato, 2002). For many composite structures additional simplified statistical measures exist, e.g., the distribution of the filament length in fibrous composites and the fiber orientation distribution function. Once this statistical data is collected, random variables can be used to evaluate numerous realizations of a virtual material. After generation of an adequate spatial discretization, the model structures can be used in computer based statistical studies. The Voronoi tessellation was found to be an efficient tool for the simulation of crystal aggregates (Kumar and Kurtz, 1994). Later, Decker and Jeulin (2000) introduced the concept of a periodic Voronoi tessellation for the use with artificial microstructures. Since, the periodic Voronoi tessellation has been applied to many microstructural problems with success (see, e.g., Barbe et al., 2001; Fritzen et al., 2009; Böhlke et al., 2010). Often the finite element method (FEM) (e.g., Zienkiewicz et al., 2006) is used in order to evaluate the mechanical and thermo-mechanical properties. The FEM requires a three-dimensional discretization of the microstructure. The construction of these discretizations from experimental data is still a challenging procedure for two-dimensional problems, see e.g., Yue et al. (2003), Prabu and Karunamoorthy (2008) or Reid et al. (2008), and often requires manual interactions. For the three-dimensional case, tools are currently being developed by various groups (Kim et al., 2002; Bhandari et al., 2007; Jang et al., 2008) for different classes of materials. The latter underlines the demand for efficient three-dimensional mesh generation methods. Therefore, the authors recently developed a generator for a particular class of periodic model microstructures based on the periodic...