Multiscale Modelling of Random Geometric Birth-and-Growth Processes, for Multi-Physics Problems Occurring in Material Sciences and Biomedicine

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Abstract: Nucleation and growth processes arise in a variety of natural and technological applications, such as solidification of materials, semiconductor crystal growth, biomineralization (shell growth), tumor growth, vasculogenesis, DNA replication. All these processes may be modelled as birth-and-growth processes (germ-grain models), which are composed of two processes, birth (nucleation, branching, etc.) and subsequent growth of spatial structures (crystals, vessel networks, etc), which, in general, are both stochastic in time and space. These structures usually induce a random division of the relevant spatial region, known as a random tessellation. A quantitative description of a random tessellation can be given, in terms of the mean volume densities of interfaces (n-facets) of the random tessellation, at different Hausdorff dimensions (cells, faces, edges, vertices). In Biology it is well known that "there is an important relationship between the form or shape of a biological structure and his function" [D'Arcy Thomson, 1917]. In Material Science it is well known that mechanical properties of the final material strongly depend on the mean densities of the interfaces. In Medicine, the understanding of the principles and the dominant mechanisms underlying processes like tumor growth or angiogenesis is an essential prerequisite for prevention and treatment. Predictive mathematical models for morphological features can contribute to the solution of optimization or optimal control problems. If the underlying field is decoupled from the nucleation and growth process, evolution equations for the relevant geometric densities can be derived in a rigorous way. A non trivial difficulty arises from the strong coupling of the kinetic parameters of the relevant birth-and-growth (or branching-and-growth) process with the underlying field, such as temperature, and the geometric spatial densities of the evolving spatial random tessellation itself. Methods for reducing complexity include homogenization at mesoscales, thus leading to hybrid models (deterministic at the larger scale, and stochastic at lower scales); we bridge the two scales by introducing a mesoscale at which we may locally average the microscopic birth-and-growth model in presence of a large number of grains. On the dual side, in order to compare numerical simulations of proposed mathematical models with existing data, we provide methods of statistical analysis for the estimation of geometric densities that characterize the morphology of a real system.

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