Random walk of Brownian particles on non-uniform grids

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Abstract

Transport of Brownian particles in a porous media or a periodic nanoscale structures is a fundamental process in bio-medicine, water treatment, pollution control and many other applications. Exact analysis of transport parameters such as effective migration speed and/or effective diffusion coefficient is still challenging, because of the complicated physics and huge varieties in different dimensions. Random walk model, due to its inherent simplicity, has been used for analyzing a large variety of systems in science, engineering, sociology, economics, humanities etc. However, when random walk model is applied to highly nonlinear systems, such as forced migration of particles in nonporous media at high Peclet number, a huge number of grids and extremely long execution time are required if we use uniform grids. To overcome this difficulty, we propose a random walk model based on non-uniform grids. The basic idea is to use high density grids in regions of high nonlinearity, or sharp changes in variables, and to adopt coarse grids in regions of smooth variations. Formulas and algorithms for forced convective diffusions are derived on the non-uniform grids in free space and with presence of boundaries. We tested the proposed algorithms using problems of given analytical results and the published benchmark results in literatures. Based on these, we analyzed migration of Brownian particles in the two-dimensional periodic nano-channel structures. The dependences of effective migration speed and effective diffusion coefficients on the external force are analyzed. The proposed algorithm provides a simple solution to the systems with high nonlinearity and/or large variation in sizes in different dimensions.

Keywords: Random walk; Nonuniform grid; Convective diffusion; Brownian particles

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