Ergodic Estimations of Upscaled Coefficients for Diffusion in Random Velocity Fields

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Abstract Upscaled coefficients for diffusion in ergodic velocity fields are derived by summing up correlations of increments of the position process, or equivalently of the Lagrangian velocity. Ergodic estimations of the correlations are obtained from time averages over finite paths sampled on a single trajectory of the process and a space average with respect to the initial positions of the paths. The first term in this path decomposition of the diffusion coefficients corresponds to Markovian diffusive behavior and is the only contribution for processes with independent increments. The next terms describe memory effects on diffusion coefficients until they level off to the value of the upscaled coefficients. Since the convergence with respect to the path length is rather fast and no repeated Monte Carlo simulations are required, this method speeds up the computation of the upscaled coefficients over methods based on long-time limit and ensemble averages by four orders of magnitude.

1 Introduction

Direct Monte Carlo estimations of diffusion coefficients by averaging over ensembles of realizations of the process and taking the large time limit often constitute a numerical challenge in simulation studies. Owing to the ergodicity of the process, the numerical burden can be reduced to a great extent.

For ergodic transport processes, the ensemble average of the observables can be estimated by the arithmetic mean of the observables resulting from repeated simulations of diffusion, done for the same realization of velocity field and for point-like

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sources with different locations uniformly distributed over large enough spatial domains [8]. Even though promising results can be obtained in this way, this "ergodic simulations method" depends on the quality of the numerically generated processes: worse are the ergodic properties of the latter, greater is the number of simulations for different initial positions required to achieve the desired accuracy. For instance, results of two-dimensional ergodic simulations of diffusion in random velocity fields presented in [8], obtained by averaging over a moderate number of 121 initial positions, indicated the approach of ergodic estimates to the corresponding ensemble averages but the accuracy of the upscaled diffusion coefficients was not yet satisfactory. To increase the accuracy, more initial positions should be considered, which would increase the computational costs and render the ergodic simulations less competitive with respect to the direct Monte Carlo approach.

The "path decomposition method" proposed in Sect. 2 provides ergodic estimates of diffusion coefficients by sums of correlations of increments on paths of increasing but finite lengths on a single trajectory of the diffusion process. To increase the accuracy, the path correlations are further averaged over a large number of paths. In the case of diffusion in random velocity fields, the upscaled diffusion coefficients can be explicitly written in terms of correlations of the Lagrangian velocity, sampled on the same trajectory (Sect. 3). Summing up autoregressive processes of order 1, diffusion processes with memory and exactly computable diffusion coefficients are constructed and are used to test the path decomposition method (Sect. 4). Finally, in Sect. 5, the new approach is applied to a problem of diffusion in random velocity fields which occurs in modeling groundwater contamination. Some conclusions are drawn in Sect. 6.

2 Path Decomposition of Diffusion Coefficients

Let $X = \{X_t, t \geq 0\}$ be a stochastic process of mean zero starting from $X_0 = 0$. If after a transient time X behaves as a normal diffusion, the diffusion coefficient is related to the expectation $E\{X_t^2\}$ by the Einstein formula [1, 15]

$$D = \lim_{t \longrightarrow \infty} \frac{1}{2t} E\{X_t^2\}. \tag{1}$$

Dividing a finite time interval $[0,t]$ in S subintervals of equal length τ, $t = S\tau$, the position X_t and its square X_t^2 can be expressed in terms of random variables $\delta X_s = X_{s\tau} - X_{(s-1)\tau}$,

$$X_t = \sum_{s=1}^{S} \delta X_s,\; X_t^2 = \sum_{s=1}^{S} (\delta X_s)^2 + 2\sum_{r=1}^{S-1}\sum_{s=1}^{S-r} \delta X_s \delta X_{s+r}.$$

Defining the (time average) correlations