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STOCHASTIC TRAJECTORY MODELS FOR TURBULENT DIFFUSION: MONTE CARLO PROCESS VERSUS MARKOV CHAINS

LIAN-PING WANG* and DAVID E. STOCK†

Department of Mechanical and Materials Engineering, Washington State University, Pullman, WA 99164-2920, U.S.A.

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Abstract—Turbulent diffusion of passive scalars and particles is often simulated with either a Monte Carlo process or a Markov chain. Knowledge of the velocity correlation generated by either of these stochastic trajectory models is essential to their application. The velocity correlation for Monte Carlo process and Markov chain was studied analytically and numerically. A general relationship was developed between the Lagrangian velocity correlation and the probability density function for the time steps in a Monte Carlo process. The velocity correlation was found to be independent of the fluid velocity probability density function, but to be related to the time-step probability density function. For a Monte Carlo process with a constant time step, the velocity correlation is a triangle function; and the integral time scale is equal to one-half of the time-step length. When the time step was chosen randomly with an exponential pdf distribution, the resulting velocity correlation was an exponential function. Other time-step probability density functions, such as a uniform distribution and a half-Gaussian distribution, were also tested.

A Markov chain, which presumes one-step memory, has a piecewise linear velocity correlation function with a finite time step. For a Markov chain with a short time step, only an exponential velocity correlation function can be realized. Thus, a Monte Carlo process with random time steps is more versatile than a Markov chain. Direct numerical calculation of the velocity correlation verified the analytical results.

A new model which combines the ideas of the Monte Carlo process and the Markov chain was developed. By examining the long-time mean square dispersion, we found an exact solution for the Lagrangian integral time scale of the new model in terms of the intercorrelation parameter and the mean and the variance of the time steps. Using this new model, we can generate any velocity correlation, including one with a negative tail. Two approximate solutions that give upper and lower bounds for the Lagrangian velocity correlation are proposed.

Key word index: Turbulent dispersion, numerical simulation, Monte Carlo process, Markov chains, Langevin equation.

1. INTRODUCTION

According to Taylor's (1921) work on "diffusion by continuous movements", the natural way to describe diffusion in a turbulent field is to follow the trajectories of fluid elements and to accumulate velocity statistics along their path. This Lagrangian approach is the basis for the two major stochastic trajectory models for turbulent diffusion and dispersion: the Monte Carlo process (Gosman and Ioannides, 1981; Shuen *et al.*, 1983; Kallio and Reeks, 1989) and the Markov chains (Durbin, 1980; Sawford, 1982, 1985; Walklate, 1987; Zhuang *et al.*, 1989). Both the Monte Carlo process and Markov chains can be viewed as a special case of Markov process (van Kampen, 1981). The Monte Carlo process generates the Lagrangian velocity through independent random numbers with either constant or random time steps, while the Markov chains simulate the Lagrangian velocity through dependent random numbers with one-step memory. Although both models have been widely used to study turbulent diffusion numerically, the Lagrangian velocity correlations embedded in these models are not well understood. A knowledge of the Lagrangian velocity corrections generated by these models is essential to their applications. In this paper, the results of a study of the Lagrangian velocity correlations generated by the stochastic trajectory models are presented.

We shall consider the diffusion of fluid elements in a homogeneous, isotropic and stationary turbulent field. Without loss of generality, a one-dimensional formulation of the diffusion relation can be used, i.e.

$$\varepsilon(t)=\frac{1}{2}\frac{\mathrm{d}\langle y^2(t)\rangle}{\mathrm{d}t}=u_0^2\int_0^t R(\tau)\mathrm{d}\tau, \qquad (1)$$

where $\varepsilon(t)$ is the diffusivity, u_0 is the root-mean-square (rms) fluctuation velocity, $y(t)$ is the displacement of a fluid element relative to its mean motion, and the angle brackets indicate an ensemble average over all realizations of the trajectories. The Lagrangian velocity autocorrelation, $R(\tau)$, is defined as

$$R(\tau)=\frac{\langle v(t)v(t+\tau)\rangle}{u_0^2}, \qquad (2)$$

* Present address: Center for Fluid Mechanics, Turbulence and Computation, Box 1966, Brown University, Providence, RI 02912, U.S.A.

† To whom correspondence should be addressed.

where $v(t)$ is the instantaneous velocity along a particle trajectory. The Lagrangian integral time, T_L, is the net area under the correlation curve,

$$T_L = \int_0^\infty R(\tau)\,d\tau, \qquad (3)$$

and is a measure of how long the particle velocity at present time will affect the future motion. In the short-time limit, Equation (1) may be written as

$$\varepsilon(t) = u_0^2 t, \quad \langle y^2(t) \rangle = u_0^2 t^2, \quad \text{for} \quad t \ll T_L. \qquad (4)$$

The long-time limit is

$$\varepsilon(t) = u_0^2 T_L, \quad \langle y^2(t) \rangle \sim 2u_0^2 T_L t, \quad \text{for} \quad t \gg T_L. \qquad (5)$$

Therefore, the diffusion statistics under the two limits are independent of the shape of $R(\tau)$. The integral time T_L is an important parameter for the long-time diffusion.

The Monte Carlo process with constant time steps is often used when long-time diffusion is of interest. It is an efficient method since the time-step size can be of the order of T_L. The Markov chains with constant time steps are known to give an exponential velocity correlation in the limit that the time step size δt approaches zero (Durbin, 1980). In a numerical simulation, this exponential correlation can be reasonably realized when $\delta t \sim 0.1 T_L$. The Markov chains have been used for short-time as well as intermediate-time ($t \sim T_L$) diffusion simulations. Recently, the Monte Carlo process with random time steps, instead of the usual constant time step, has also been used for diffusion simulations (Kallio and Reeks, 1989). The use of random time steps seems logical since the size of a turbulent eddy and its lifetime are both random. The Lagrangian velocity corrections embedded in such a general Monte Carlo process has not been studied. Markov chains can also be extended to allow for random time steps.

The integral equation of diffusion (Smith, 1982; Pasquill and Smith, 1983) can also be used to model the diffusion process. This technique requires that the Lagrangian scales be known or that they be approximated. It has the advantage of being simple to formulate, fast to compute, and capable of calculating the moments of the concentration distribution directly in terms of prescribed Lagrangian scales. The purpose of our paper, however, is to show how the Lagrangian scales are related to the parameters used in a stochastic model. Our goal is to understand how to adjust the parameters to obtain a desired Lagrangian correlation.

In this work, we obtained the Lagrangian velocity correlation for a Monte Carlo process by transforming the ensemble average into time average for a stationary random process and employing physical reasoning to find the contribution of individual velocity pairs to the velocity correlation function. The same method was used to study the Lagrangian velocity correlation for a Markov chain with random time steps. The analytical results were verified by numerical tests.

2. VELOCITY CORRELATION IN MONTE CARLO PROCESS

2.1. *Monte Carlo process with constant time steps*

The velocity of a particle in a Monte Carlo (or random walk) process with constant time steps is given by

$$v(0 \to T) = v_1, \quad v(T \to 2T) = v_2,$$
$$v(2T \to 3T) = v_3, \ldots\ldots, \qquad (6)$$

where $v_1, v_2, v_3, \ldots$, are random numbers of zero mean. The variance of v_i is assumed to be u_0^2, the mean square fluctuation velocity of the flow; T is the size of time steps.

The velocity correlation for this *discontinuous* stochastic process can be obtained as follows. Since for a stationary ergodic random process the ensemble average can be replaced by a time average over one trajectory, Equation (2) for the velocity correlation can be written as

$$R(\tau) = \lim_{t \to \infty} \int_0^t \frac{v(t')v(t'+\tau)}{u_0^2}\,dt'. \qquad (7)$$

The time average of the product of velocity pairs with time separation τ is of interest. One can easily see that the velocity correlation is zero for all $\tau \geq T$, since the two velocities in the pair are independent. For $\tau < T$, a velocity pair has $(T-\tau)/T$ chance to be equal and in this portion of time the velocity correlation between the pair is one (Fig. 1). Thus we have

$$R(\tau) = \frac{T-\tau}{T}, \quad \text{for } \tau < T;$$
$$R(\tau) = 0, \quad \text{for } \tau \geq T. \qquad (8)$$

This is a triangle function.

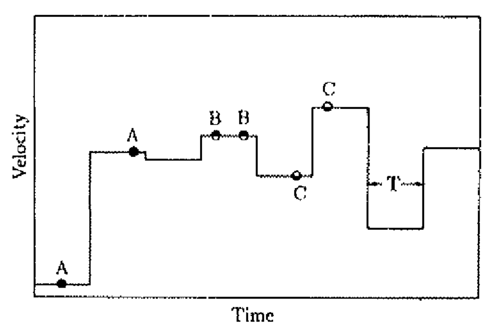

Fig. 1. A sketch showing correlation for individual velocity pairs: the velocity pair A–A has no correlation since the time delay (τ) is larger than the time-step size (T); the velocity pair B–B has a correlation of one since both points are located in the same time step; the correlation for pair C–C is zero since the two points are located in different time steps, although the time delay is less than T.

We can also numerically calculate the velocity correlation by taking a large number of the discrete velocity samples from the velocity history. Figure 2 shows a velocity history, $v(t)$, based on Equation (6) (solid line) and the corresponding velocity samples, $v(k\tau)$, $k=1, 2, 3, \ldots$, for $\tau=0.4T$ (symbols). The value $R(\tau)$ can be directly calculated by

$$R(\tau)=\frac{1}{Nu_0^2}\sum_{i=1}^{i=N} v(i\tau)v(i\tau+\tau), \tag{9}$$

where N is the number of velocity pairs used in the correlation estimation. Figure 3 compares the analytical result, Equation (8), with the result of a numerical calculation based on Equation (9). The good agreement indicates that the triangle function is the correct correlation function. Numerical calculations of the velocity correlation using probability distributions other than Gaussian distribution for v_i give the same result, implying that the velocity correlation $R(\tau)$ is independent of the form of probability distribution used for the velocity value.

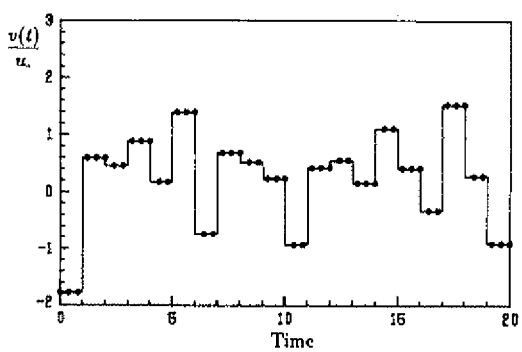

Fig. 2. A velocity history generated by the Monte Carlo process with constant time steps and the corresponding velocity samples with an interdata time of $0.4T$. Gaussian deviates were used for the velocity values at different time steps. The number of velocity pairs in the samples depends on both the total record length and the interdata time.

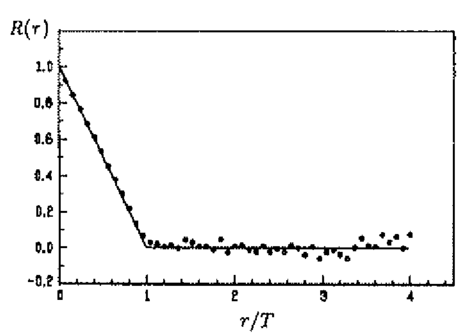

Fig. 3. Velocity correlation for the Monte Carlo process with constant time steps: solid line shows the analytical result (triangle function) and symbols represent the result of direct numerical calculation. In the numerical calculation, a total record length of $3000T$ was used.

Now it is interesting to examine diffusion statistics. The integral time scale is obviously $\frac{1}{2}\times 1\times T$ (the area under the correlation curve). Therefore, if we simply set $T=T_L$, with T_L the real Lagrangian integral scale of a fluid particle, the integral time scale of the velocity signal generated by the Monte Carlo process will be $T_L/2$. The long-time diffusivity is then $u_0^2 T_L/2$, one-half the true long-time diffusivity (see Equation 5). This was referred to as the self-consistency problem by Kallio and Reeks (1989) in their simulation. Here we see clearly why this occurs. The self-consistency can be achieved simply by allowing the time-step length T to be $2T_L$.

2.2. *Monte Carlo process with random time steps*

If instead of using a constant time step we can assume that the time steps are random with a probability density distribution

$$p(t_i)=f(t_i)>0, \quad \text{for } t_i\geqslant 0,$$
$$p(t_i)=0, \quad \text{for } t_i<0; \tag{10}$$

and generate the velocity signal as

$$v(0\to t_1)=v_1,\ v(t_1\to t_1+t_2)=v_2,$$
$$v(t_1+t_2\to t_1+t_2+t_3)=v_3,\ldots\ldots, \tag{11}$$

where $v_1, v_2, v_3, \ldots$, are independent random numbers with *any* probability density distribution, as long as the mean is zero and the variance is the rms fluctuating velocity of the flow. A Monte Carlo process with constant time steps can be viewed as a special case of (10) and (11) with $f(t_i)=\delta(t_i-T)$. An example of velocity history for a Monte Carlo process with random time steps is shown in Fig. 4.

To find the velocity autocorrelation for the general Monte Carlo process, we first notice the following (Fig. 5): (1) the velocity history in any time interval with $t_i<\tau$ does not contribute to the velocity correlation $R(\tau)$, since velocity values in different time intervals are independent; (2) the velocity history in time intervals with $t_i>\tau$ has $R(\tau)$ equal to one for a $t_i-\tau$

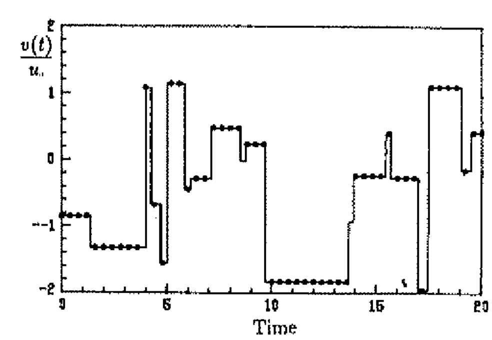

Fig. 4. Velocity history (solid line) generated by the Monte Carlo process with exponential deviates as time-step size. The symbols represent the velocity samples of interdata time equal to $0.4T$, which were used to calculate directly the correlation value with a time delay equal to $0.4T$, i.e. $R(\tau=0.4T)$.

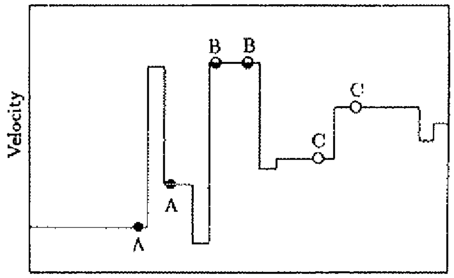

Fig. 5. A sketch showing the contribution of velocity history for individual time step to the correlation value at a given time delay: all the three velocity pairs, A–A, B–B and C–C, have the same time delay but only the B–B pair has a contribution to the velocity correlation. A–A has a zero correlation since the time-step size in between the pair is less than the given time delay. C–C has no correlation since the two points are located in different time steps, although the time-step size in the neighborhood of the pair is larger than the time delay.

duration and zero for the remaining duration. Therefore, Equation (7) becomes

$$R(\tau)=\sum_{i,\text{ such that } t_i>\tau}(t_i-\tau)\Big/\sum_{\text{all } i}t_i. \qquad (12)$$

Dividing both the numerator and the denominator of the right-hand side of Equation (12) by the number of time intervals, n, and letting n go to infinity gives

$$R(\tau)=\frac{\int_{\tau}^{\infty}(t_i-\tau)f(t_i)\,\mathrm{d}t_i}{T}, \qquad (13)$$

where T is the mean of the time interval t_i

$$T=\int_0^{\infty}t_i f(t_i)\,\mathrm{d}t_i. \qquad (14)$$

Equation (13) directly relates the Lagrangian velocity autocorrelation (characteristics of turbulent diffusion) to the pdf function of the time-step size, $f(t_i)$, in the Monte Carlo process (characteristics of the model). Since $f(t_i)$ is always non-negative, Equation (13) indicates that the velocity correlation is always non-negative for the generalized Monte Carlo process. We also notice that the form of pdf function for v_i does not affect the velocity correlation since it does not appear in the relation. In addition, if $R(\tau)$ is continuous and differentiable, we may express $f(t_i)$ in terms of the velocity correlation function as

$$f(t_i)=T\left.\frac{\mathrm{d}^2R(\tau)}{\mathrm{d}\tau^2}\right|_{\tau=t_i}. \qquad (15)$$

Equation (15) shows what $f(t_i)$ to use if a given velocity correlation is to be generated.

We must now show how to relate the mean value of t_i, T, to the Lagrangian time scale, T_L, in order to ensure the self-consistency of the model. Substituting Equation (13) into Equation (3) and performing partial integration with respect to τ, we obtain

$$2TT_L=\int_0^{\infty}t_i^2f(t_i)\,\mathrm{d}t_i. \qquad (16)$$

The right-hand side of (16) is the mean square of the time-step size. Table 1 lists the velocity correlation and $T-T_L$ relation for four different $f(t_i)$ distributions.

It is interesting to see that exponential velocity correlation can be generated by a Monte Carlo process with an exponential distribution for the time-step size. In this case the self-consistency is retained by simply using $T=T_L$. For the other three $f(t_i)$ distributions, T is different from T_L. Using Equation (16), we can show that $0<T\leqslant 2T_L$.

Figures 6a, 6b and 6c compare the analytical results with the results of direct numerical calculations of the Lagrangian velocity correlation. Good agreement is seen for all the distributions tested.

3. VELOCITY CORRELATION FOR A MARKOV CHAIN

3.1. *A Markov chain with finite time steps*

A Markov chain simulates the velocity history with a one-step memory. The velocity values between two adjoining time steps have an intercorrelation of ρ, and the velocity history is given by

$$\left.\begin{aligned} v(0\to t_1)&\to v_1=u_0v_1'\\ v(t_1\to t_1+t_2)&=v_2=\rho v_1+u_0\sqrt{1-\rho^2}\,v_2'\\ v(t_1+t_2\to t_1+t_2+t_3)&=v_3=\rho v_2+u_0\sqrt{1-\rho^2}\,v_3' \end{aligned}\right\}, \qquad (17)$$

where v_1', v_2', v_3', ..., are independent random numbers with zero mean and unit variance. The value of ρ

Table 1. Examples of the generalized Monte Carlo process

	$f(t_i)$	$R(\tau)$	T–T_L relation
Constant	$\delta(t_i-T)$	$1-\tau/T$, for $\tau<T$ 0, otherwise	$T=2T_L$
Uniform	$1/2T$, for $0<t_i<2T$ 0, otherwise	$(1-\tau/2T)^2$, for $\tau<2T$ 0, otherwise	$T=1.5T_L$
Exponential	$(1/T)\exp(-t_i/T)$	$\exp(-\tau/T)$	$T=T_L$
Half-Gaussian	$(2/T\pi)\exp(-t_i^2/\pi T^2)$	$\exp(-\tau^2/\pi T^2)-(\tau/T)$ $\times[1-\mathrm{erf}(\tau/\sqrt{\pi}T)]$	$T=\frac{4}{\pi}T_L$

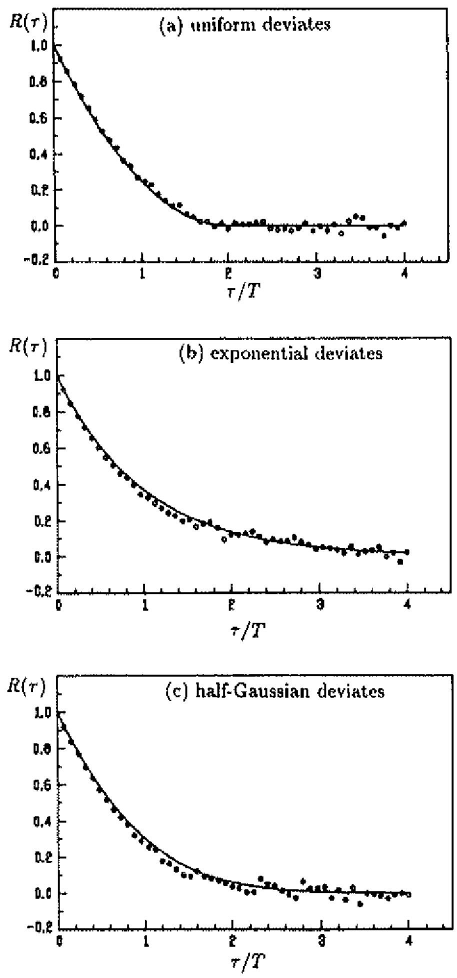

Fig. 6. Velocity correlations for the Monte Carlo process for various time-step pdf: solid line shows the analytical result, Equation (13), and symbols represent the results of direct numerical calculation. In the numerical calculations, 3000 time steps were used.

may depend on the length of the time step. It then follows that

$$\langle v_i v_i \rangle = u_0^2, \quad \langle v_i v_{i+1} \rangle = \rho u_0^2,$$
$$\langle v_i v_{i+2} \rangle = \rho^2 u_0^2, \quad \ldots.. \tag{18}$$

Figure 7 shows an example of velocity history for a Markov chain with constant and finite time steps.

If the time steps, $t_1, t_2, t_3, \ldots$, are constant and equal to T, then it can be shown, using the same methodology as discussed in the last section, that the exact velocity correlation is

$$R(\tau, T) = \rho^m[1 + (\rho - 1)(\tau/T - m)],$$
$$\text{for } m \leqslant \tau/T < m + 1;$$
$$m = 0, 1, 2, 3 \ldots \tag{19}$$

A numerical test of this relation is shown in Fig. 8. A Markov chain with a finite time step produces a

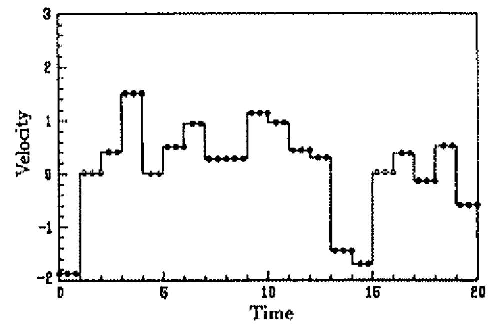

Fig. 7. Velocity history (solid line) generated by a Markov chain with $\rho = 0.6$. The symbols represent the corresponding velocity samples of interdata time equal to $0.4T$.

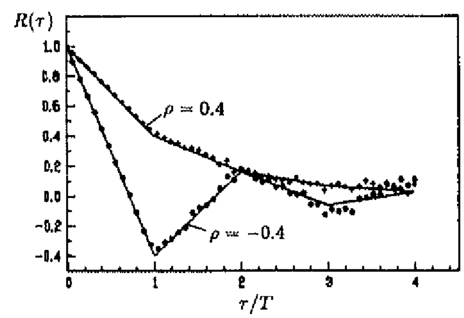

Fig. 8. Velocity correlations for Markov chains with finite time steps: solid line shows the analytical result, Equation (19), and symbols represent the results of direct numerical calculation. In the numerical calculations, 3000 time steps were used.

piecewise linear correlation function. The integral time scale is $T_L = (T/2)(1+\rho)/(1-\rho)$, which is a function of both the time-step size and the intercorrelation parameter.

3.2. *Markov chain with short time steps*

A Markov chain with short time steps has been used to simulate atmospheric diffusion. To be complete, we now show that Equation (19) will reduce to an exponential function and that the Lagrangian integral time is independent of the time-step size used as the time-step size becomes small.

When the time-step size T goes to zero, the velocity intercorrelation parameter ρ approaches one. Therefore, we let

$$\rho = 1 - \beta T, \tag{20}$$

where β is a parameter. If $T \to 0$, Equation (19) reduces to

$$R(\tau = nT) = \lim_{n\to\infty,\, T\to 0} (1 - \beta T)^n$$
$$= \lim_{n\to\infty} \left(1 - \frac{\beta\tau}{n}\right)^n = \exp(-\beta\tau). \tag{21}$$

The integral time is $1/\beta$. Therefore, the parameter β is nothing but $1/T_L$. Letting $dt \equiv T$ and using (20) for ρ with $\beta = 1/T_L$, we can write Equation (17) as

$$dv \equiv v_{i+1} - v_i = -\frac{v_i}{T_L}\,dt + u_0\sqrt{\frac{2}{T_L}}\,dw_i, \qquad (22)$$

when $dt \to 0$. Here dw_i is any independent random number (white noise) of zero mean and variance equal to dt. Equation (22) is known as the Langevin equation and has been extensively used to model atmospheric diffusion (Durbin, 1980; Sawford, 1982). It is often stated that $dt \equiv T$ should be less than $0.1T_L$ to ensure no significant influence of the time-step size on the Lagrangian velocity correlation (convergence and consistency). We can check the difference between the true correlation (Equation 19) and the convergent correlation when $dt \to 0$ (Equation 21). For $dt = 0.1T_L$ and $\tau = T_L$, the exact value of $R(\tau) = (19/21)^{10} = 0.36757$. The convergent value is $R(\tau) = e^{-1} = 0.36788$. Therefore a time step of $0.1T_L$ is small enough to ensure convergence and consistency.

4. VELOCITY CORRELATION FOR THE MARKOV CHAIN–MONTE CARLO MODEL

Constant time steps are used in the Markov chains, but we can extend the idea of the Markov chains by allowing the time steps to be random numbers with some pdf function, as was assumed in the generalized Monte Carlo process. We call this method of simulating the Lagrangian velocity by combining Equation (17) and Equation (10) the Markov chain–Monte Carlo model, which is more general than either the Markov chain or Monte-Carlo process discussed in the previous sections. Figure 9 shows an example of the velocity history for this new model. The velocity correlations for the model are developed in this section.

We have not been able to develop an exact solution for the velocity correlation for the Markov chain–Monte Carlo model. However, we find the following two approximations. The usefulness and accuracy of the approximations will be examined by comparing them with direct numerical calculations.

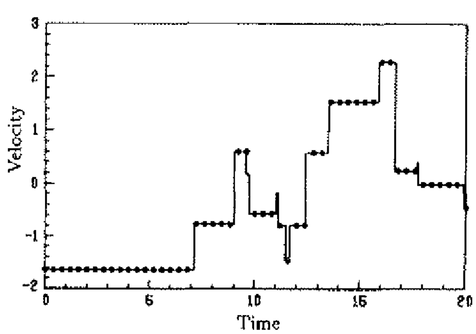

Fig. 9. Velocity history (solid line) generated by the Markov chain–Monte Carlo model with $\rho = 0.6$. Exponential random deviates were used for the time-step size. The symbols represent the corresponding velocity samples of interdata time equal to $0.4T$.

A first approximation was constructed by weighting the Markov chain correlation for uniform time steps (Equation 19) with the time step pdf, $f(t_i)$. The correlation for each time step, $R(\tau, t_i)$, are weighted by the fraction of the total time for which this size of step is taken, $t_i f(t_i)$. Therefore, we can approximate the velocity correlation as

$$R(\tau) = \frac{\int_0^{\infty} R(\tau, t_i)\, t_i f(t_i)\,dt_i}{\int_0^{\infty} t_i f(t_i)\,dt}. \qquad (23)$$

Substituting Equation (19) for $R(\tau, t_i)$ into (23) and simplifying, we have

$$R(\tau) = \frac{1}{T}\sum_{j=0}^{\infty}\int_{\frac{\tau}{j+1}}^{\frac{\tau}{j}} \rho^j[t_i - (1-\rho)(\tau - jt_i)]\,f(t_i)\,dt_i. \qquad (24)$$

This approximation assumes that time steps of the same values occur at the same time. This indirectly impose some correlations on the time steps. The results of this approximation for the four different $f(t_i)$ distributions listed in Table 1 are given in Appendix A.

A second approximation was developed by modifying the correlation for the generalized Monte Carlo process (Equation 13), by a factor of $\exp(\rho\tau/T)$:

$$R(\tau) = \exp(\rho\tau/T)\,\frac{\int_\tau^{\infty}(t_i - \tau) f(t_i)\,dt_i}{T}. \qquad (25)$$

The exponential factor is used since the convergent correlation for Markov chains is exponential.

Figures 10a to 10d compare the two approximations with direct numerical calculations of velocity correlations. Several comments are in order. First, both approximations give the correct value for the velocity correlation when $\rho = 0$, which is expected since the new model reduces to the Monte Carlo process. Second, when the time steps are constant, the first approximation is exact while the second approximation gives a poor prediction; however, when the time steps are exponential deviates, the second approximation is an exact solution (Appendix B). Third, the first approximation is better than the second approximation when time steps are uniform deviates. Fourth, in the case of half-Gaussian time steps, the numerical data are in between the two approximations. Fifth, the first approximation tends to overpredict correlation when $\rho > 0$ and underpredict correlation when $\rho < 0$; the second approximation does the opposite. Sixth, a smooth and negative loop in the velocity correlation can be generated by our new model.

Although the exact solution for the velocity correlation for our new model is not known, the exact solution to the Lagrangian integral time can be obtained by directly examining the long-time mean

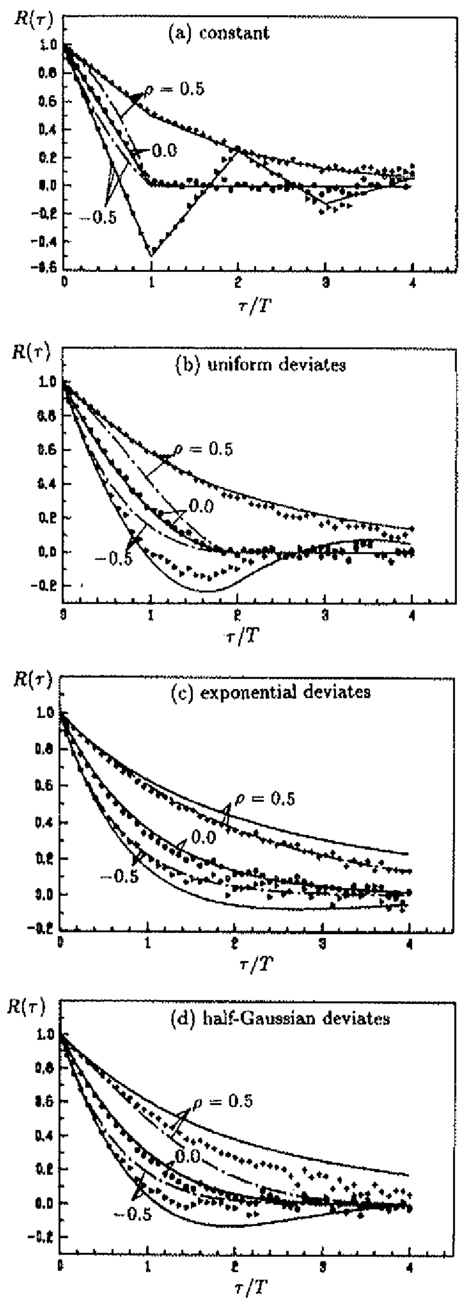

Fig. 10. Velocity correlations for the Markov chain–Monte Carlo model: solid line shows the first analytical approximation, Equation (24), dashed line shows the second analytical approximation, Equation (25), and symbols represent the results of direct numerical calculation. In the numerical calculation, 3000 time steps were used.

square displacement (Appendix C). The value T_L is found to be related to three model characteristic parameters: the mean value of t_i, the mean square of t_i and the velocity intercorrelation; i.e.

$$T_L = \frac{\langle t_i^2 \rangle}{2T} + T\frac{\rho}{1-\rho}. \tag{26}$$

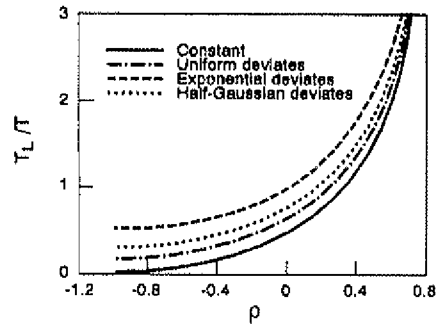

Fig. 11. Lagrangian time scales in the Markov chain–Monte Carlo model with different pdf distribution functions for the time step.

Figure 11 shows a Lagrangian time scale for the different $f(t_i)$ distributions. The ratio T_L/T increases monotonically with ρ. An exponential distribution gives the largest value for T_L/T, while a constant time step gives the smallest T_L/T.

The new model has more capability for modeling turbulent diffusion than either the Markov chain or the Monte Carlo process since it is possible for the new model to generate any desired velocity correlation function by adjusting the intercorrelation ρ or the time-step pdf function, $f(t_i)$. The proper model characteristics can be determined by numerical tests. The two approximations for the velocity correlation can be used as a guide to help pick the model characteristics. Random time steps should be used if a smooth correlation function is to be produced. Negative ρ can be used in the model if a negative correlation loop is required.

5. CONCLUSIONS

The Lagrangian velocity correlation is the most important characteristic of a stochastic trajectory model when it is used to simulate turbulent diffusion. Our analytical results show that the Monte Carlo process with constant time steps has a triangle correlation function. A Monte Carlo process with random time steps can generate many smooth positive correlation functions, including the exponential function. On the other hand, Markov chains with a constant and finite time step give a piecewise linear correlation function which depends on both the velocity intercorrelation and the time-step size. In the limit of a short time step, the exponential function is the only consistent and convergent correlation. Therefore, a Monte Carlo process with random time steps is more versatile for turbulent diffusion modeling than a Markov chain. In addition, by using a Monte Carlo process to replace a Markov chain in numerical models of atmospheric turbulent diffusion, the computation time can be remarkably reduced, since the time-step size for a Monte Carlo process can be of the order of the Lagrangian integral time.

We have also developed a new model which extends the idea of the Markov chain to allow for the use of random time steps. Proper choice of the model characteristics enables the new model to produce any smooth velocity correlation, including the one with a negative tail. The new model widens the applicability of stochastic trajectory model. We recommend that further work be done to test the new model as well as the Monte Carlo process with random time steps for atmospheric turbulent-diffusion modeling.

It is desired to explore further the physical implication of the pdf function, $f(t_i)$, for the time-step size in a stochastic trajectory model, since $f(t_i)$ is the backbone of the model. The use of a correct $f(t_i)$ makes the model more realistic. If possible, experimental data should be gathered for the pdf function. The time-step pdf function may be related to the distribution of the lifetime for turbulent eddies. The relationship, if any, between the intercorrelation and the time-step pdf function should also be studied.

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APPENDIX A
THE FIRST APPROXIMATION OF VELOCITY CORRELATION FOR THE MARKOV CHAIN-MONTE CARLO MODEL

When the pdf distribution for the time steps is known, Equation (24) can be simplified to give an approximation for the velocity correlation. Here we present the results for the four $f(t_i)$ distributions listed in Table 1.

1. *Constant time steps*

$$R(\tau, T)=\rho^m[1+(\rho-1)(\tau/T-m)],$$
$$\text{for } m\leqslant \tau/T<m+1;$$
$$m=0, 1, 2, 3\ldots.$$

2. *Uniform deviates*

$$R(\tau)=\rho^m\left\{1+m-\rho m-(1-\rho)\frac{\tau}{T}+\frac{\tau}{4T^2}\left[\frac{1-\rho}{m+1}-\frac{\rho}{(m+1)^2}\right]\right\}$$
$$+\frac{\tau^2}{T^2}\sum_{j=m+1}^{\infty}\left(\frac{1}{j}+\frac{\rho}{j+1}\right)\frac{1}{j(j+1)}\frac{\rho^j}{4},$$
$$\text{for } m<\frac{\tau}{2T}<m+1;\ m=0, 1, 2, 3\ldots.$$

3. *Exponential deviates*

$$R(\tau)=(1-\rho)^2\sum_{j=1}^{\infty} j\rho^{j-1}\exp\left(-\frac{\tau}{jT}\right).$$

4. *Half-Gaussian deviates*

$$R(\tau)=\sum_{j=0}^{\infty}\rho^j\left\{(1+j-j\rho)\left[\exp\left(-\frac{\tau^2}{\pi T^2(j+1)^2}\right)\right.\right.$$
$$\left.-\exp\left(-\frac{\tau^2}{\pi T^2 j^2}\right)\right]-(1-\rho)\frac{\tau}{T}\left[\operatorname{erf}\left(\frac{\tau}{\sqrt{\pi}\,T_i}\right)\right.$$
$$\left.\left.-\operatorname{erf}\left(\frac{\tau}{\sqrt{\pi}\,T(j+1)}\right)\right]\right\},$$

where erf(x) is the standard error function.

APPENDIX B
THE EXACT SOLUTION FOR VELOCITY CORRELATION

Although we are unable to obtain an explicit and closed-form solution for the velocity correlation in Section 4 for the Markov Chain–Monte Carlo model, the exact velocity correlation can be written formally as

$$R(\tau)=\frac{1}{T}\int_{\tau}^{\infty}(t-\tau)\,dt\sum_{k=1}^{\infty}\rho^{k-1}f_k(t). \tag{B1}$$

In arriving at (B1), we applied a similar argument to that used for Equation (13); $f_k(t)$ is the pdf function for $t_1+t_2+\ldots+t_k=t$, subject to the requirement that $t_1+t_2+\ldots+t_k+t_{k+1}<\tau$. Therefore

$$f_1(t)=f(t),$$
$$f_2(t)=\int_0^{\tau} dt_1\, f(t_1)f(t-t_1)$$
$$f_3(t)=\int_0^{\tau} dt_1\int_0^{\tau-t_1} dt_2\, f(t_1)f(t_2)f(t-t_1-t_2),$$

for $t\geqslant\tau$. In general, it is very difficult to find $f_k(t)$ explicitly. However, for the exponential pdf, $f(t)=1/T\exp(-t/T)$, it can be shown that

$$f_k(t)=\frac{\tau^{k-1}\exp(-t/T)}{(k-1)!\,T^k}. \tag{B2}$$

Substituting (B2) into (B1), we have

$$R(\tau)=\exp\left(-\frac{(1-\rho)\tau}{T}\right), \tag{B3}$$

which is exactly the same as Equation (25).

APPENDIX C
THE INTEGRAL TIME SCALE FOR THE MARKOV CHAIN–MONTE CARLO MODEL

Here we explain how to obtain an exact solution to the integral time scale for the Markov chain–Monte Carlo model by simply studying the long-time mean square displacement.

We first note that the relative displacement after n steps is

$$y(n)=u_1t_1+u_2t_2+u_3t_3+\ldots\ldots+u_nt_n. \quad \text{(C1)}$$

Then the mean square value is

$$\langle y^2(n)\rangle = nu_0^2\langle t_i^2\rangle + 2u_0^2T^2[(n-1)\rho+(n-2)\rho^2 + (n-3)\rho^3+\ldots+\rho^{n-1}]. \quad \text{(C2)}$$

The following have been used in obtaining (C2):

$$\langle t_it_j\rangle=\langle t_i\rangle\langle t_j\rangle=T^2, \quad \text{for } i\neq j$$
$$\langle u_1u_2\rangle=\langle u_2u_3\rangle=\ldots=\rho u_0^2$$
$$\langle u_1u_3\rangle=\langle u_2u_4\rangle=\ldots=\rho^2u_0^2$$
$$\langle u_1u_4\rangle=\langle u_2u_5\rangle=\ldots=\rho^3u_0^2$$

and so on.

Equation (C2) can be rewritten as

$$\langle y^2(n)\rangle = nu_0^2\langle t_i^2\rangle + 2T^2u_0^2\left(\frac{\rho}{1-\rho}\right)\left(n-1-\frac{\rho-\rho^n}{1-\rho}\right). \quad \text{(C3)}$$

Now if we assume n is very large, then the total time would be $t=\Sigma_{i=0}^{n}t_i\sim nT$. We have

$$\langle y^2(t)\rangle = u_0^2\left(\frac{\langle t_i^2\rangle}{T}+2T\frac{\rho}{1-\rho}\right)t, \quad t\gg T. \quad \text{(C4)}$$

Also notice that

$$\langle y^2(t)\rangle \sim 2u_0^2T_Lt, \quad t\gg T. \quad \text{(C5)}$$

Compare (C4) and (C5), we have

$$T_L=\frac{\langle t_i^2\rangle}{2T}+T\frac{\rho}{1-\rho}. \quad \text{(C6)}$$

Thus we see that the integral time scale is only related to the mean square of time steps, the mean of t_i, and the velocity intercorrelation ρ. For the four $f(t_i)$ distributions listed in Table 1, the $T-T_L$ relations are given in the following.

1. *Constant time steps*

$$\langle t_i^2\rangle = T^2$$
$$T_L=\left(\frac{1+\rho}{1-\rho}\right)\frac{T}{2}.$$

2. *Uniform deviates*

$$\langle t_i^2\rangle=\frac{4}{3}T^2$$
$$T_L=\left(\frac{2+\rho}{1-\rho}\right)\frac{T}{3}.$$

3. *Exponential deviates*

$$\langle t_i^2\rangle = 2T^2$$
$$T_L=\frac{T}{1-\rho}.$$

4. *Half-Gaussian deviates*

$$\langle t_i^2\rangle=\frac{\pi}{2}T^2$$
$$T_L=\left(\frac{\pi+(4-\pi)\rho}{1-\rho}\right)\frac{T}{4}.$$