"Rogue Velocities" in a Lagrangian Stochastic Model for Idealized Inhomogeneous Turbulence

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A Lagrangian stochastic model may sometimes generate velocities of unrealistic magnitude, and several authors have taken ad hoc steps to control their impact. The occurrence of these "rogue velocities" would, on first sight, appear to contradict the model's being well mixed; however, the problem is typically experienced in the context of a complex (and in some cases, discontinuous, i.e., gridded) regime of turbulence, corresponding to which there may (implicitly) be limitations on the allowable size of the time step that had not been respected. This article seeks to observe rogue velocities in an artificial regime of 1-D turbulence, in which two regions of differing constant velocity variance are joined by a ramp such that the gradient in velocity variance is discontinuous. The evolution of an initially well-mixed distribution of tracer is computed by integrating the Chapman-Kolmogorov equation (the resulting calculation is compared with the corresponding stochastic solution). It is found that unless the time step is small relative to an inhomogeneity time scale implied by the field of Eulerian velocity statistics, the well-mixed condition is violated: large velocities occur with greater probability than they ought.

1. INTRODUCTION

Yee and Wilson [2007] summarized instances where well-mixed Lagrangian stochastic (LS) models have been reported to generate excessive velocities and suggested the cause is twofold: an intrinsic instability of the generalized Langevin equations whose triggering (or otherwise) hinges on particularities of the velocity statistics and is liable to occur in complex flows, and the stiffness of the generalized Langevin equations, due to which simple integration schemes result in growing round-off errors. Without suggesting that hypothesis is incorrect, this article revisits the question of the causation of rogue velocities by asking whether, in effect, they originate because the time step dt fails to satisfy (perhaps unrecognized) limitations that are implicit in the velocity statistics (in LS simulations for complex flows, it is rarely feasible to decrease the model time step sufficiently to eliminate rogue velocities). The objective is to take an extremely simple regime of inhomogeneous turbulence, to determine, analytically if possible, whether rogue trajectories occur and (if so) to establish whether this can be attributed to an excessively large time step.

2. IDEALIZED 1-D TURBULENCE

Consider a 1-D regime of turbulence: motion along the unbounded coordinate x with Eulerian velocity u, with the restriction that u is Gaussian with zero mean and has the variance profile

$$\sigma_u^2 = \begin{cases} \sigma_1^2 & x < -D/2, \\ \sigma_1^2 + \alpha(x + D/2) & |x| \le D/2, \\ \sigma_2^2 & x > D/2, \end{cases} \tag{1}$$

where $\alpha = (\sigma_2^2 - \sigma_1^2)/D$. The Eulerian velocity variance is a continuous function of x with discontinuities in slope at the

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two ends of the ramp region, and the probability density function (PDF) for velocity is

$$g_a(u|x) = \frac{1}{\sqrt{2\pi}\,\sigma_u(x)} \exp\left(-\frac{u^2}{2\sigma_u^2(x)}\right). \tag{2}$$

The turbulent kinetic energy dissipation rate ϵ is constant, and the ratio $\sigma_u{}^2/\varepsilon$ implies a turbulence time scale. The geometry and the inhomogeneity of the velocity statistics imply further time scales, e.g., $\tau_D = D/\sigma_u$ and $\tau_D{}^* = D/\Delta\sigma_u$ (where $\Delta\sigma_u = |\sigma_2 - \sigma_1|$).

3. WELL-MIXED LS MODEL

The above prescription of the Eulerian statistics implies a unique well-mixed, first-order LS model for the evolution of the position and velocity (X,U) of a fluid element [*Thomson*, 1987], specifically

$$\mathrm{d}X = U\ \mathrm{d}t, \tag{3}$$

$$\mathrm{d}U = a_u(X, U)\ \mathrm{d}t + \sqrt{C_0\epsilon}\ \mathrm{d}\xi, \tag{4}$$

$$a_u = -\frac{C_0\epsilon}{2\sigma_u^2} U + \frac{1}{2}\frac{\partial\sigma_u^2}{\partial x}\left(1 + \frac{U^2}{\sigma_u^2}\right), \tag{5}$$

where $\mathrm{d}t$ is the time increment, C_0 the dimensionless universal constant appearing in Kolmogorov's similarity law for the second-order Lagrangian velocity structure function, and $\mathrm{d}\xi$ is an uncorrelated Gaussian signal with $\overline{\mathrm{d}\xi} = 0$ and $\overline{\mathrm{d}\xi^2} = \mathrm{d}t$. Note that the systematic part of the acceleration (a_u) is undefined at $x = \pm D/2$; wherever an LS model is "driven" by a gridded flow field, such discontinuities are likely to be prevalent and may be universal (continuity has no meaning for a gridded flow field). For convenience, define $B \equiv C_0\epsilon/2$.

4. TEST FOR RETENTION OF WELL-MIXED STATE

Let $p(x, u, t)$ be the joint probability density function for the position and velocity at time t of a fluid element that, at $t = 0$, was released at random on the x axis with its velocity chosen randomly from the Eulerian velocity PDF pertaining to that point. The objective is to compute $p(x, u, t)$, then extract the marginal PDF (p_x) for particle position and the conditional PDF (p_u) for particle velocity at a *given* position, namely,

$$p_x(x, t) = \int_{u=-\infty}^{\infty} p(x, u, t)\ \mathrm{d}u, \tag{6}$$

$$p_u(u, t|x) = \frac{p(x, u, t)}{p_x(x, t)}. \tag{7}$$

Ideally, these should not differ from the initial uniform distribution in space and the given inhomogeneous Gaussian in velocity (equation (2)), and here we will test whether this is the case after a single finite time step, i.e., at $t = \Delta t$.

The Chapman-Kolmogorov equation demands that

$$p(x, u, \Delta t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p_{1|1}(x, u, \Delta t|x_0, u_0, 0) \times p(x_0, u_0, 0)\ \mathrm{d}x_0\mathrm{d}u_0, \tag{8}$$

where $p_{1|1}(\cdot|\cdot)$ is the transition density corresponding to the chosen stochastic model, and the initial value of p here satisfies

$$p(x_0, u_0, 0) = c\ g_a(u_0|x_0) \tag{9}$$

with c = const. The transition density corresponding to equations (3)–(5) is

$$p_{1|1}(x, u, \Delta t|x_0, u_0, 0) = \frac{\delta(x - x_0 - u_0\Delta t)}{\sqrt{2\pi}\sqrt{2B\Delta t}} \times \exp\left(-\frac{[u - u_0 - a_u(x_0, u_0)\ \Delta t]^2}{4B\Delta t}\right) \tag{10}$$

[*Wilson and Flesch*, 1993; *Rodean*, 1996, Section 11.4], and in view of the delta-function equation (8) simplifies to

$$p(x, u, \Delta t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}u_0}{\sqrt{2\pi\sigma_u^2(x - u_0\Delta t)}} \times \exp\left(\frac{-u_0^2}{2\sigma_u^2(x - u_0\Delta t)}\right)\frac{1}{\sqrt{2\pi}\sqrt{2B\Delta t}} \times \exp\left(\frac{-[u - u_0 - a_u(x - u_0\Delta t, u_0)\Delta t]^2}{4B\Delta t}\right). \tag{11}$$

With the substitution $q = u_0 - x/\Delta t$, this integral may be split into three parts, namely,

$$2\pi\sqrt{2B\Delta t}\quad p(x, u, \Delta t) = I_1 + I_2 + I_3, \tag{12}$$

where

$$I_1 = \frac{1}{\sigma_2}\int_{-\infty}^{-D/(2\Delta t)} \exp\left(-\frac{q^2 + 2qx/\Delta t + (x/\Delta t)^2}{2\sigma_2^2}\right) \times \exp\left(-\frac{[u - q - x/\Delta t + \Delta t B(q + x/\Delta t)/\sigma_2^2]^2}{4B\Delta t}\right)\mathrm{d}q, \tag{13}$$

$$I_3 = \frac{1}{\sigma_1} \int_{D/(2\Delta t)}^{\infty} \exp\left(-\frac{q^2 + 2qx/\Delta t + (x/\Delta t)^2}{2\sigma_1^2}\right)$$

$$\times \exp\left(-\frac{[u - q - x/\Delta t + \Delta t B(q + x/\Delta t)/\sigma_1^2]^2}{4B\Delta t}\right) dq, \quad (14)$$

and

$$I_2 = \int_{-D/(2\Delta t)}^{D/(2\Delta t)} \frac{1}{\sqrt{\sigma_1^2 + \alpha(-q\Delta t + D/2)}} \exp\left(\frac{-\eta^2}{4B\Delta t}\right)$$

$$\times \exp\left(-\frac{q^2 + 2qx/\Delta t + (x/\Delta t)^2}{2(\sigma_1^2 + \alpha(-q\Delta t + D/2))}\right) dq, \quad (15)$$

with

$$\eta = u - q - \frac{x}{\Delta t} + \frac{B\Delta t\ (q + x/\Delta t)}{\sigma_1^2 + \alpha(-q\Delta t + D/2)} - \frac{\alpha \Delta t}{2}\left(1 + \frac{(q + x/\Delta t)^2}{\sigma_1^2 + \alpha(-q\Delta t + D/2)}\right). \quad (16)$$

There appears little prospect of integrating I_2 analytically; therefore, all three integrals have here been evaluated numerically. These approximate solutions (of the Chapman-Kolmogorov equation) have also been compared with the outcome of stochastic (random flight) solutions, with which, despite the approximations of numerical procedure, they have proven consistent.

5. RESULTS

Solutions will be shown for the case $D = 10^{-1}$ m, $\sigma_1^2 = 1$ m^2 s^{-2}, $\sigma_2^2 = 2$ m^2 s^{-2}, $C_0\epsilon = 1$ m^2 s^{-3}. The joint density function $p(x, u, \Delta t)$ has been evaluated at the discrete points defined by

$$x = -0.5 \ldots 0.5, \quad \Delta x = 0.05 \text{ m},$$
$$u/\sigma_u = -6 \ldots 6, \quad \Delta u/\sigma_u = 0.05.$$

The numerical integration was performed with

$$q = -10^4 \ldots 10^4, \quad \Delta q = 0.001 \text{ m s}^{-1} \quad (17)$$

(tests with smaller values proved that the outcomes to be shown are effectively independent of Δx, $\Delta u/\sigma_u$, and Δq).

For the chosen parameter values, the Lagrangian decorrelation time scale $\tau_L = 2\sigma_u^2/(C_0\epsilon)$ is of order 1 s, while the inhomogeneity time scales $\tau_D = D/\sigma_u$ and τ_D^* are of order 0.1 s and so represent a more stringent limit on the acceptable value of the time step. We may expect $p(x, u, \Delta t)$ to be well mixed provided $\Delta t << 0.1$ s ($\approx D/\sigma_u$).

Figure 1 gives the solution for $\Delta t = 0.001$ s ($<<D/\sigma_u$) and confirms this expectation: there is negligible change in the

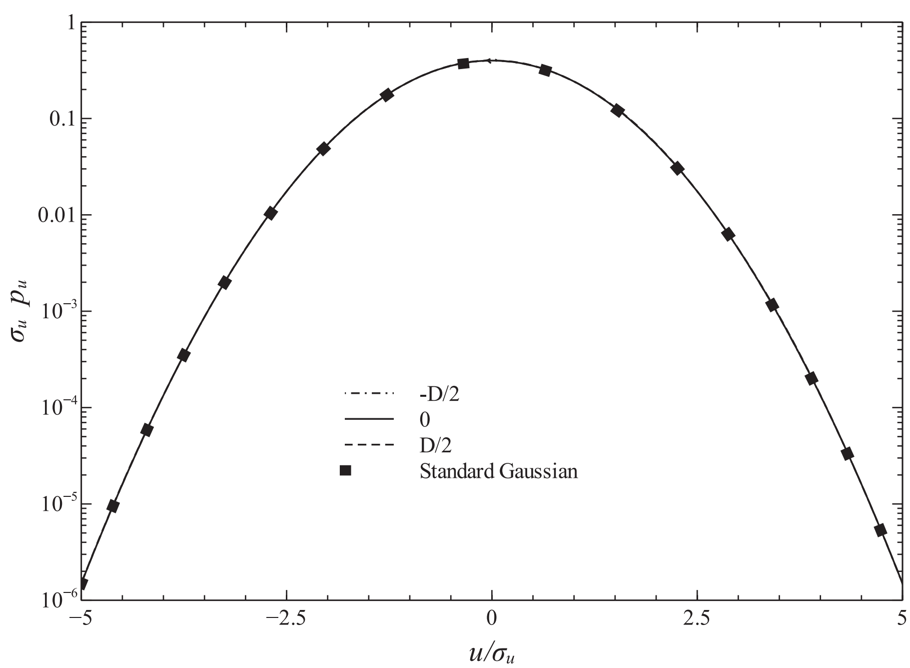

Figure 1. Normalized velocity probability density functions (PDFs) ($\sigma_u p_u$ versus u/σ_u) after a single time step $\Delta t = 0.001$ ($<<D/\sigma_u$), compared with the standardized Gaussian. The PDFs at $x = -D/2$, 0, $D/2$ are masked by the initial Gaussian, and PDFs at all other tested locations ($|x| \leq 0.5$) were equally indistinguishable from the initial state.

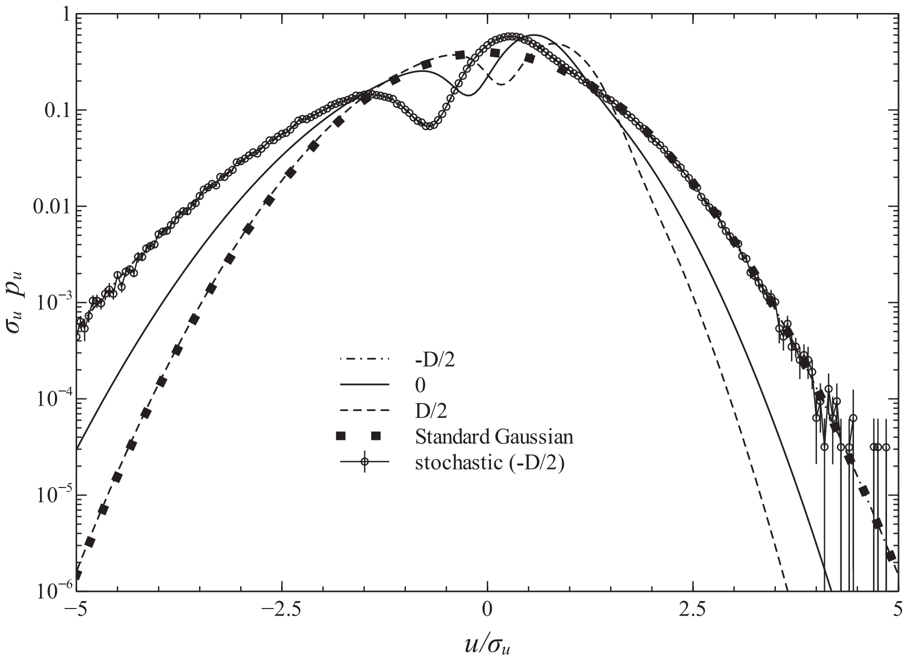

Figure 2. Normalized velocity PDFs ($\sigma_u p_u$ versus u/σ_u) after a single time step $\Delta t = 0.1$ ($\approx D/\sigma_u$), compared to the standardized Gaussian. (The stochastic solution is plotted for location $x/D = -0.5$, with error bars designating ± 1 standard error).

velocity PDF (and density: not shown). Figure 2 contrasts the outcome when $\Delta t = 0.1$ s, such that $\Delta t \approx D/\sigma_u << \tau_L$. There are large percentage changes in the velocity PDFs relative to the original Gaussian; for example, at $x = -D/2$ the frequency of large negative velocities $u/\sigma_u = -5$ is increased by more than two orders of magnitude (relative to the initial probability at that point).

As indicated in Figure 2, this outcome (for the velocity PDF) is consistent with an alternative calculation, namely, a random flight solution of equations (3)–(5) forward over a single time step. For the latter, each of N_p-independent stochastic trajectories was initialized at a random point on the domain $|x| \leq S$, where $S >> D$ (for the specific simulation shown $S = 5$ m and $D = 0.1$ m), with a random velocity

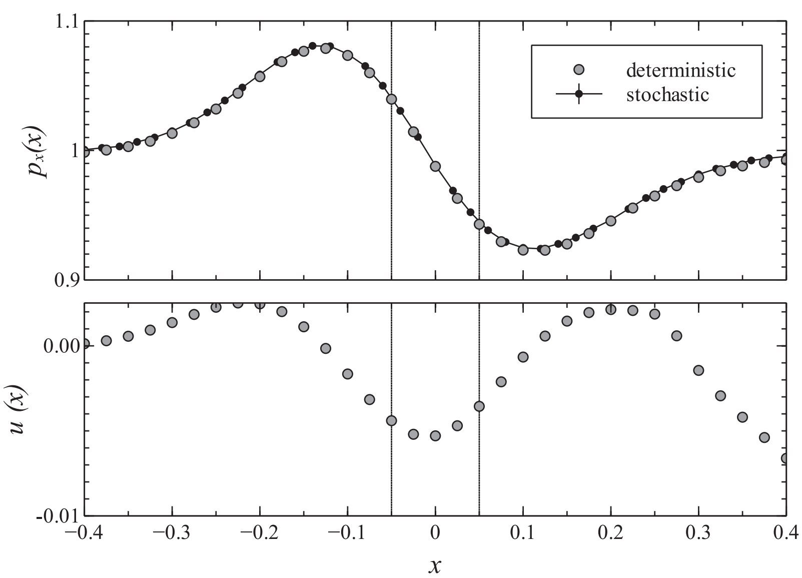

Figure 3. Marginal PDF for (top) position and (bottom) the mean velocity, after a single time step $\Delta t = 0.1$ ($\approx D/\sigma_u$).

consistent with equation (2) at that point. Particle position was updated first (without restriction, i.e., particles were not confined to the initial domain), followed by velocity. After this single step, histograms of particle velocity (normalized as u/σ_u; bin width $\Delta u/\sigma_u = 0.05$) were sampled at chosen points x or, more specifically, within narrow slices $x \pm 0.001$ m of the x axis. Interestingly, rogue velocities *did* occur in the stochastic simulation, albeit rarely: there were six occurrences of a rogue velocity (defined as a deviation from the local mean velocity exceeding six standard deviations) in a total of $N_P = 19 \times (1.6 \times 10^8)$ trajectories. Figure 3 gives the mean density and mean velocity profiles corresponding to the deterministic and stochastic simulations, which consistently indicate about a 10% disturbance to each profile (i.e., density and velocity).

6. CONCLUSION

This is perhaps the simplest first-order LS model and the simplest regime of turbulence reported to have resulted in rogue velocities. In this case, it seems plausible to state that the cause is no more subtle than the use of a time step whose magnitude is excessive, relative to an inhomogeneity time scale that is implicit in the turbulence regime under study.

Rogue trajectories may be tolerable in the context of simulations oriented toward predicting the mean concentration field, upon which (by virtue of their rarity), it may be that they have no appreciable influence. However, they present a serious difficulty for LS micromixing models computing higher moments of concentration [e.g., *Postma et al.*, 2012]. Some authors "reset" particle velocity (with a random choice from the Eulerian velocity PDF) whenever it has exceeded some (large) multiple of the local standard deviation. Another intervention (E. Fattal, personal communication, 2012) is to restore the offending particle to the position in position-velocity space it had occupied prior to its attaining its excessive velocity and to recompute the path with a reduced time step.

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