Accurate Integration of Stochastic Climate Models with Application to El Niño

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ABSTRACT

Numerical models are one of the most important theoretical tools in atmospheric research, and the development of numerical techniques specifically designed to model the atmosphere has been an important discipline for many years. In recent years, stochastic numerical models have been introduced in order to investigate more fully Hasselmann's suggestion that the effect of rapidly varying ''weather'' noise on more slowly varying ''climate'' could be treated as stochastic forcing. In this article an accurate method of integrating stochastic climate models is introduced and compared with some other commonly used techniques. It is shown that particular care must be used when the size of rapid variations in the ''weather'' depends upon the ''climate.'' How the implementation of stochasticity in a numerical model can affect the detection of multiple dynamical regimes in model output is discussed.

To illustrate the usefulness of the numerical schemes, three stochastic models of El Niño having different assumptions about the random forcing are generated. Each of these models reproduces by construction the observed mean and covariance structure of tropical Indo-Pacific sea surface temperature. It is shown that the skew and kurtosis of an observed time series representing El Niño is well within the distributions of these statistics expected from finite sampling. The observed trend, however, is unlikely to be explained by sampling. As always, more investigation of this issue is required.

1. Introduction

Numerical stochastic models have recently become rather common in weather and climate research. This is seen by an online search of titles published by the American Meteorological Society: of 133 articles with the word ''stochastic'' in the title (as of March 2002), more than a fourth appeared in the last five years. The purpose of using a stochastic climate model, of course, is to represent rapidly varying processes that cannot be resolved on deterministic time scales but that are nevertheless necessary for an accurate depiction of a dynamical system. Following Hasselmann's (1976) suggestion that this might be done, stochastic numerical models have been used to diagnose the dynamical behavior of such multiscale physical systems as El Niño (e.g., Chang et al. 1996; Thompson and Battisti 2000, 2001), the response of midlatitude ocean dynamics to local weather forcing (e.g., Alexander and Penland 1996), and storm-track dynamics (Whitaker and Sardeshmukh 1998). Stochastic parameterizations of unresolved processes in numerical prediction models have also been investigated as a way to improve estimates of predictability in ensemble forecasts (Buizza et al. 1999; Palmer 2001). Given the large number of stochastic modeling studies, we hope the authors of them will forgive us for not mentioning all of them here.

Dynamically consistent methods of stochastic parameterizations are not arbitrary but are dictated by the dynamical form of the central limit theorem (CLT). The CLT has been described elsewhere (Sardeshmukh et al. 2001a), and although we do not repeat that discussion here, we remind the reader that a dynamically consistent

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parameterization cannot be devised without knowing (or, at least, guessing) something about the real spectral properties of the process to be parameterized. That is, application of the central limit theorem requires an explicit estimation of the temporal covariance properties both of the macroscopic system to be investigated and, somewhat counterintuitively, the perturbing influence one wishes to treat as white noise. Practical details may be found in Khasminski'i (1966), Majda et al. (1999), and Sardeshmukh et al. (2001a). An oceanographic example may be found in Penland (1985).

In this article, we assume that the researcher has already applied the CLT, has been satisfied that the time scales of the multiscale system allow a dynamically consistent stochastic parameterization in terms of white noise, has derived the appropriate stochastic differential equations (SDEs) to be integrated in the numerical model, and has decided which set of calculus rules is required by the physical system at hand. Generally speaking, if a system is smooth enough to allow application of the CLT, it is likely that the traditional rules of Riemann calculus apply. That is, when the stochastic parameterization is meant to represent a continuous, highly chaotic system such as turbulent eddy feedbacks in fluid flow, familiar rules of calculus are appropriate and are called ''Stratonovich.'' Another set of calculus rules (''Itô'' calculus) is obeyed by systems that are only approximately continuous. Rainfall, which falls in individual drops but is nevertheless parameterized with a differential equation, *may* be an example of an Itô system. Whether a system should be modeled as Itô or Stratonovich depends on what modelers would do with an infinite amount of computer resources. If, in such an idealistic case, we would start off with differential equations of motion and not need any randomness at all because we could temporally resolve all chaotic interactions, we would choose Stratonovich calculus in the numerical model with realistic time steps. If, at infinitesimal time scales, we could resolve the delay between one occurrence of a random process and the next, we might choose Itô calculus to solve the differential-equations representing that process in our numerical model. Please note that the appropriate calculus is decided by the continuity properties of the *real system* and *not* by those of our numerical discretization of it. If the real system is microscopically continuous (i.e., Stratonovich), we have to cheat the discrete numerical model into *acting* as though it were continuous.

The important issue here is that we are not free to choose which calculus is appropriate for a given project. Itô calculus is often appropriate in data assimilation projects where the noise is due to independent, discrete errors, and, indeed, the Stratonovich integral does not even exist in some nonlinear filtering projects (Jazwinski 1970). Alternatively, incorrect application of the Itô integral to a physically Stratonovich system is likely to produce skewed results.

It is, at least in principle, possible to transform a Stratonovich differential equation into an Itô equation and vice versa. Consider the following general Stratonovich SDE:

$$d\mathbf{x} = \mathbf{F}(\mathbf{x}, t)dt + \mathbf{G}(\mathbf{x}, t) \circ d\mathbf{W}, \tag{1a}$$

where $\mathbf{x}$ is the stochastic process of interest, t is time, $\mathbf{W}$ is a vector of independent Wiener processes (Gardiner 1985; Penland 1996), $\mathbf{F}(\mathbf{x}, t)$ is a vector function of $\mathbf{x}$ and t, and $G_{i\alpha}$, an element of the matrix $\mathbf{G}(\mathbf{x}, t)$, is a function of $\mathbf{x}$ and t and multiplies the αth Wiener process. In accordance with standard mathematical notation, the symbol $\circ$ denotes that integration over the Wiener process is to be performed in the sense of Stratonovich. Equation (1a) is equivalent to the following Itô SDE:

$$dx_j = \left\{F_j(\mathbf{x}, t) + \frac{1}{2}\sum_{i\alpha=1} \frac{\partial G_{j\alpha}}{\partial x_i} G_{i\alpha}\right\}dt + \sum_{\alpha=1} G_{j\alpha}dW_\alpha. \tag{1b}$$

The first summation term in Eq. (1b) is called the ''noise-induced drift'' or the ''Itô correction'' and, if $\mathbf{G}(\mathbf{x}, t)$ is known and easily differentiated, it is easy to transform the description of a physical system in one calculus to the description of that same physical system in the other. Unfortunately, this transformation is generally impossible to effect in practice, underscoring the necessity of deciding in advance which calculus is appropriate for the physical system to be simulated. Note that the equations are equivalent if $\mathbf{G}$ is independent of $\mathbf{x}$, that is, if the system is an ''additive noise process.''

Rather than reproduce the rules of Itô calculus here, we refer the reader to one of the many excellent textbooks (e.g., Arnold 1974; Gardiner 1985; Kloeden and Platen 1992) on the subject. Stratonovich calculus, we repeat, follows the familiar rules of Riemann. The problem for the numerical modeler of a stochastic system is that standard deterministic algorithms for integrating differential equations may converge to neither one nor the other if, indeed, they converge at all (Rümelin 1982). Compounding the problem is the fact that an inappropriate integration scheme can yield results that look reasonable, agree with physical intuition, and yet be completely—or, worse, partially—spurious. The only way out of this depressing state of affairs is to use only those numerical schemes that have been proven to converge to one or the other physically realizable calculus. A collection of well-researched stochastic integration schemes is found in the textbook by Kloeden and Platen (1992, KP92 hereafter).

It is unlikely that climate researchers will rewrite complex numerical models in order to incorporate properly sanctioned numerical schemes for stochastic integration. Simply adding a stochastic term to existing computer code, on the other hand, may introduce large undetectable errors, including the possibility of spurious dynamical regimes. The most desirable situation, then, seems to be for mathematicians to examine extant climate models and devise legitimate methods of stochastic integration that require a minimum of revising the computer code. The motivation of this article was to find a numerical scheme by which stochastic forcing could be introduced into a barotropic vorticity model. This model is, perhaps, the simplest meteorologically relevant numerical model, but many of the numerical issues involved in making it stochastic are also relevant to the most complex general circulation models (GCMs). Further, the stochastic barotropic model has versions that are simple enough for the mean response to be evaluated analytically, thus allowing verification of numerical techniques. Several such schemes have recently been developed by Ewald and Temam (2003a,b, ET03, meaning the pair of articles, hereafter). However, even the simple barotropic vorticity model is too complex to exhibit in isolation each of the numerical issues we wish to illustrate, and, besides, it does not show off all the advantages of the newly developed scheme. For this reason, we have chosen two *very* simple systems to introduce two of the schemes introduced in ET03 to the meteorological community. The first, a one-dimensional genic model (Horsthemke and Lefever 1984), describes a dynamical system with a finite range of values and two stable, noise-induced dynamical regimes. This example shows the ability of an explicit scheme (called ET03a hereafter) to reproduce the stationary probability distribution function (pdf) of a system whose multiple regimes result from the state-dependent stochastic forcing. The second example consists of a univariate diffusion equation with constant deterministic forcing and stochastically varying damping. An implicit scheme (called ET03b hereafter) is exhibited here, echoing the structure of the barotropic vorticity equation. The functional form of the stationary pdf is known in both examples, allowing easy verification of the techniques. Although both examples presented here are Stratonovich systems, we provide guidance in the modeling of Itô systems as well.

Among the important issues of introducing new numerical schemes is whether or not it can play a useful role in solving meteorological problems. We demonstrate the usefulness of these schemes by investigating whether or not the observed skew and kurtosis in the distribution of sea surface temperatures (SSTs) in the El Niño region of the Pacific is indicative of nonlinear dynamics, or if the observed statistics may be explained by sampling. Using a linear inverse model (LIM) of Indo-Pacific SST (Penland and Magorian 1993; Penland and Matrosova 1994; Penland and Sardeshmukh 1995), we generated synthetic SST time series for that region using linear dynamics driven by additive Gaussian white noise. By construction, this model reproduces the covariance structure of the observed SSTs. However, significant skew and kurtosis (Wilks 1962) in the observations would suggest the existence of nonlinear dynamics or, at least, a state-dependent variance of the stochastic forcing, that is, multiplicative noise. In this study, we present results from an ensemble of models using additive and multiplicative stochastic forcing showing that the sampled skew and kurtosis of an observed El Niño time series [specifically, that corresponding to the leading empirical orthogonal function (EOF) of tropical Indo-Pacific SST] are well within the distribution of the sampled statistics obtained when the dynamical assumptions of LIM are numerically modeled. However, while the size of the sampled trend of the observed time series is insignificant at the 5% level, it is indeed significant at the 10% level, suggesting an external source of deterministic forcing.

The article is constructed as follows: Section 2 introduces ET03a and ET03b and relates them to the barotropic vorticity model. Section 3 compares the performance of ET03a with another commonly used Stratonovich stochastic integrator through consideration of the stochastic genic model. An example using ET03b is introduced in section 4. We also show in section 4 what happens when stochasticity is naively introduced and numerically integrated using algorithms valid in the deterministic case. The integration schemes are then employed in section 5 to investigate the significance of skew, kurtosis, and trend in an El Niño time series. The article ends with a discussion of stochastic integration, differences between the schemes introduced here and other commonly used integration schemes, how the physical problem dictates choice of calculus, and the relevance all this has to climate modeling.

2. Two stochastic integration schemes

Consider a stochastic differential equation that may be interpreted in the sense of either Itô or Stratonovich:

$$d\mathbf{x} = \mathbf{F}(\mathbf{x}, t)dt + \mathbf{G}(\mathbf{x}, t)d\mathbf{W}. \quad (2)$$

For many years, the standard integration techniques used by physical scientists to integrate Eq. (2) have been the Euler method if the system is Itô or additive and the Heun method if the system is Stratonovich (Rümelin 1982; KP92). For a time step Δ, the Euler method converges to Itô calculus with global error of order $\Delta^{1/2}$. The Heun method, which is a second-order Runge–Kutta method, has been shown by Rümelin (1980, 1982) to converge to Stratonovich calculus with a one-time-step error of order $\Delta^{1/2}$ or Δ, depending on the structure of the noise. At first glance this is good news; it appears that the scheme that may be more accurate is appropriate to the calculus we might most often require, and even if we require Itô calculus we can use the more accurate scheme if $\mathbf{G}(\mathbf{x}, t)$ is simple enough to apply the Itô correction. Unfortunately, as discussed by KP92, the Heun scheme does not converge *regularly* with Δ; that is, the results do not improve uniformly with decreasing time step. In practical problems this disadvantage negates any increase in formal accuracy.

There does exist an algorithm, the Mil'shtein scheme (Mil'shtein 1974; KP92), which with suitable modifications converges to the desired stochastic calculus with error of order Δ. Both Itô and Stratonovich versions of this scheme require analytical evaluation of the Itô correction and so were quite difficult to implement for a complicated $\mathbf{G}(\mathbf{x}, t)$ until KP92 published discretized variants of them. However, these discretized variants are very computer intensive, requiring multiple evaluations of the integrand.

The ET03a method of integrating Eq. (2) is much more efficient for complicated, multidimensional integrands, and also converges with error of order Δ. The method is as follows: Let $\{z_{\gamma n}\}$ be random numbers sampled independently at time t_n from a centered Gaussian distribution with variance equal to Δ. Then, the process $\mathbf{x}$ is updated from time t_n to time t_{n+1} as

$$\begin{aligned} x_i(t_{n+1}) &= x_i(t_n) + F_i(\mathbf{x}, t_n)\Delta \\ &\quad + \sum_{l\gamma\mu} G_{l\gamma}(\mathbf{x}, t_n) \\ &\quad \times [G_{i\mu}(\mathbf{x} + \alpha_l \hat{\mathbf{e}}_l \sqrt{\Delta}, t_n) - G_{i\mu}(\mathbf{x}, t_n)] I_{(\gamma\mu),n}/(\alpha_l \sqrt{\Delta}) \\ &\quad + \sum_{\gamma} G_{i\gamma}(\mathbf{x}, t_n) z_{\gamma n}, \end{aligned} \tag{3}$$

where $\hat{\mathbf{e}}_l$ is a unit vector corresponding to the component x_l. As in the Mil'shtein scheme (KP92),

$$I_{(\gamma,\gamma),n} = (z_{\gamma n}^2 - \Delta)/2 \tag{4a}$$

for Itô calculus and

$$I_{(\gamma,\gamma),n} = z_{\gamma n}^2/2 \tag{4b}$$

for Stratonovich calculus. For $\gamma \neq \mu$, the stochastic cross terms may be approximated as in KP92 (section 5.8) or Gaines and Lyons (1994) to retain accuracy of order Δ. This, however, can be complicated. If somewhat larger error can be tolerated, then, as in the Mil'shtein scheme for either Itô or Stratonovich calculus, we approximate

$$I_{(\gamma,\mu),n} = z_{\gamma n} z_{\mu n}/2. \tag{4c}$$

The vector parameter $\boldsymbol{\alpha}$ has units and magnitude of $\mathbf{x}/\sqrt{t}$ and allows the modeler to accommodate the discretized derivatives with respect to $\{x_l\}$ in the Itô correction to the physical problem at hand.

As shown above, ET03a is useful in many contexts. However, most global models in meteorology involve an implicit scheme. For example, a version of the barotropic vorticity equation (Sardeshmukh and Hoskins 1988) is

$$\frac{d\varsigma}{dt} = -\boldsymbol{\nabla} \cdot (\boldsymbol{\upsilon}\varsigma) + S - r\xi - \kappa\nabla^4\xi, \tag{5}$$

where ς is the total vorticity, ξ is the relative vorticity, $\boldsymbol{\upsilon}$ is the horizontal velocity, S is the Rossby wave source, r is the Newtonian damping, and κ is the diffusion coefficient. Defining F as $-\boldsymbol{\nabla}\cdot(\boldsymbol{\upsilon}\varsigma)$ and casting Eq. (5) in terms of spherical harmonics, we have

$$\frac{d\zeta_n^m}{dt} = -F_n^m + S_n^m - r\xi_n^m - \kappa\left[\frac{n(n+1)}{a_e^2}\right]\xi_n^m, \tag{6}$$

where a_e is the radius of the earth. Note that this equation is at least two-dimensional since the spherical harmonics are complex, and we revert to our usual notation of indicating vectors in bold face in what follows. The deterministic version of this equation is usually integrated numerically, first using a leapfrog step, followed by an implicit step, as in Sardeshmukh and Hoskins (1988). The stochastic analog of this procedure follows here.

First, let us simplify the notation in Eq. (5) in such a way that the following will also hold for similar types of equations. Let $\mathbf{a}_1 = -F + S$ and $\mathbf{a}_2 = -r\boldsymbol{\xi} - \kappa\nabla^4\boldsymbol{\xi}$. We now consider a stochastic differential equation of the form

$$d\boldsymbol{\xi} = [\mathbf{a}_1(t, \boldsymbol{\xi}) + \mathbf{a}_2(t, \boldsymbol{\xi})]dt + \mathbf{G}(t, \boldsymbol{\xi})d\mathbf{W}. \tag{7}$$

The implicit leapfrog scheme of Ewald and Temam (2003a,b) with time step Δ is as follows:

$$\begin{aligned} \boldsymbol{\xi}_1(t_{n+2}) &= \boldsymbol{\xi}(t_n) + 2\mathbf{a}_1(t_{n+1}, \boldsymbol{\xi}(t_{n+1}))\Delta + \mathbf{M}_n(\boldsymbol{\xi}(t_n)) \\ &\quad + \mathbf{M}_{n+1}(\boldsymbol{\xi}(t_{n+1})), \end{aligned} \tag{8a}$$

$$\boldsymbol{\xi}(t_{n+2}) = \boldsymbol{\xi}_1(t_{n+2}) + 2\mathbf{a}_2(t_{n+2}, \boldsymbol{\xi}(t_{n+2}))\Delta, \tag{8b}$$

with the ith component of the vector $\mathbf{M}_n$ defined as

$$\begin{aligned} M_{\text{in}}(\mathbf{y}) &= \sum_{l\gamma\mu} G_{l\gamma}(\mathbf{y}, t_n)\frac{\partial G_{i\mu}(\mathbf{y}, t_n)}{\partial y_l} I_{(\gamma,\mu)} \\ &\quad + \sum_{\gamma} G_{i\gamma}(\mathbf{y}, t_n) z_{\gamma n}, \end{aligned} \tag{8c}$$

and with $z_{\gamma n}$ and $I_{(\gamma,\mu)n}$ defined above. In Eq. (8c), as in the explicit case, the derivative with respect to the argument y_l is estimated as

$$\begin{aligned} &\frac{\partial G_{i\mu}(\mathbf{y}, t_n)}{\partial y_l} \\ &\quad = \frac{G_{i\mu}(\mathbf{x} + \alpha_l \hat{\mathbf{e}}_l \sqrt{\Delta}, t_n) - G_{i\mu}(\mathbf{x}, t_n)}{\alpha_l \sqrt{\Delta}}, \end{aligned} \tag{8d}$$

with the parameter α_l having units and magnitude of $y_l/\sqrt{\Delta}$.

3. Example 1: The explicit scheme

The explicit ET03a scheme is well illustrated using a version of the stochastic genic model (Arnold et al. 1978; Horsthemke and Lefever 1984):

$$dx = [½ - x]dt + \sigma x(1 - x) \circ dW, \tag{9}$$

where the symbol $\circ$ denotes that stochastic integration is to be performed in the sense of Stratonovich and where σ is a scalar parameter. The stationary probability density of this system is

$$p_s(x) = Nx^{-1}(1 - x)^{-1} \exp[-x^{-1}(1 - x)^{-1}/\sigma^2], \tag{10}$$

which is always normalizable in the interval [0, 1] with the normalization constant

$$N = \tfrac{1}{2}\exp(2/\sigma^2)K_o^{-1}(2/\sigma^2) \qquad (10b)$$

involving the modified Bessel function K_o. For $\sigma^2 < 4$, p_s is unimodal with a single maximum at $x_e = 0.5$. For $\sigma^2 > 4$, p_s is bimodal, with maxima at $x_\pm = 0.5[1 \pm (1 - 4/\sigma^2)^{1/2}]$ and one minimum at x_e. Note that without any stochastic forcing the bimodality would not exist.

We consider a system with a very shallow minimum by choosing $\sigma = 2.75$. Equation (9) was numerically integrated using the Heun method for a variety of time steps Δ between 0.0001 and 0.1. The integration was begun using an initial condition of $x = x_e$, and, after a suitable spinup to allow the integration to forget the initial condition, 100 000 samples separated by a sampling interval of $t_{samp} = 0.1$ were recorded. Gaussian random deviates were generated using a Box–Mueller algorithm (Press et al. 1992) applied to uniformly distributed random numbers obtained from a Mersenne twister (Matsumoto and Nishimura 1998). The resulting stationary pdf is compared with Eq. (10) in Fig. 1a. The procedure was repeated using ET03a with $\alpha = 1$ [Eqs. (3) and (4b)] and the resulting pdf from that calculation is shown in Fig. 1b. The divergence of the Heun-integrated solution from the true solution at small time steps is clear. Even worse, this divergence is not systematic as Δ inreases or decreases.

It does appear in Fig. 1 that, in this case, the Heun method may provide a more accurate pdf than ET03a at larger time steps. The problem, of course, is that for an arbitrary physical problem one cannot know *in advance* what size time steps Heun requires in order to give results within a specified error tolerance, or even if such time steps exist. With ET03a, any loss of accuracy with decreasing time step may be traced to round-off error rather than to a problem endemic to the scheme itself.

It is the univariate nature of our example and the fact that the constant coefficients in Eq. (9) are of order one that caused us to choose $\alpha = 1$. The strength of $\boldsymbol{\alpha}$ becomes most apparent in multivariate cases involving variables obeying complicated evolution equations and whose tendencies are of different orders of magnitude. Then, it has been shown by ET03 that expensive matrix calculations can be replaced by a constant vector $\boldsymbol{\alpha}$.

4. Example 2: The implicit scheme

We give an example of using the implicit ET03b by considering a simple type of forced diffusion equation:

$$\frac{dx}{dt} = (k^2 - r)x + F. \qquad (11)$$

In Eq. (11), k and F are constant while r has a stochastic component, $r = r_o + r_s\eta$, where η is white noise. More precisely,

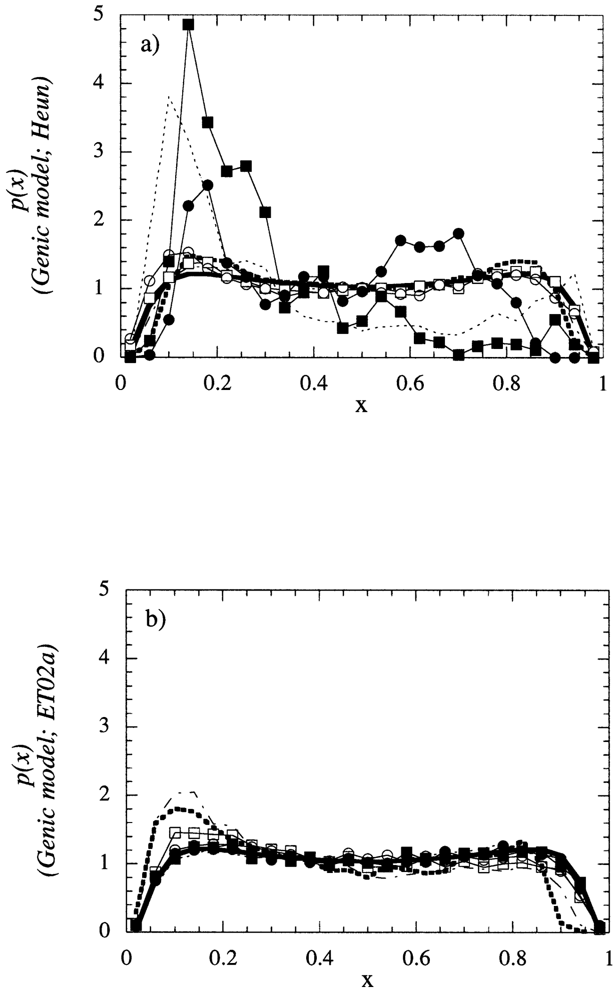

FIG. 1. (a) Probability density function estimated from numerically integrating the genic model [Eq. (9)] using the Heun method with different time steps. Heavy solid line denotes the theoretical pdf. Heavy dotted line: $\Delta = 0.1$; dot–dash: $\Delta = 0.05$; open squares: $\Delta = 0.01$; open circles: $\Delta = 0.005$; light dotted line: $\Delta = 0.001$; filled circles: $\Delta = 0.0005$; and filled squares: $\Delta = 0.0001$. (b) As in (a), but using the ET03a.

$$r\,dt = r_o\,dt + r_s\,dW. \qquad (12)$$

The corresponding Fokker–Planck equation is easily solved for the stationary pdf:

$$p_s(x) = Nx^{\beta-1}\exp(-2F/r_s^2 x), \qquad (13a)$$

where

$$\beta = 2(k^2 - r_o)/r_s^2, \qquad (13b)$$

and where the normalization constant

$$N = (2F/r_s^2)^{-\beta}/\Gamma(-\beta) \qquad (13c)$$

involves the Gamma function Γ. Note that $\beta < 0$ if Eq. (11) has a stable stationary solution. For $F > 0$, $p_s(x)$ is unimodal with x confined to the positive real axis and $p_s(0) = 0$.

In our experiment, we take $k = 0.1$, $r_o = -0.51$, r_s

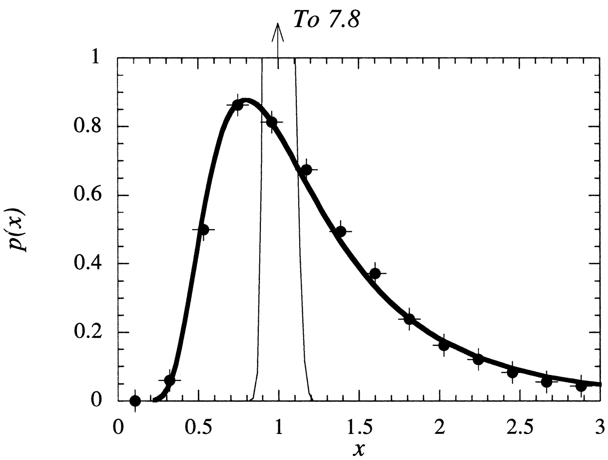

FIG. 2. Probability density function estimated from integrating Eq. (11). Heavy solid line denotes the theoretical pdf. Filled circles denote the ET03b scheme using $\alpha = 1$. Crosses denote ET03b scheme using $\alpha = 0.5$. Light solid line denotes the traditional method.

$= 0.5$, and $F = 0.5$. We define $a_1 = F$ and $a_2 = (k^2 - r_o)x$. The integration is begun at the peak of p_s at $x_p = 0.862$ with a time step of $\Delta = 0.005$. We again spin the model up enough to forget the initial condition, after which 10 000 samples are recorded at a sampling interval of $t_{\rm samp} = 0.1$. Two values of the parameter α, $\alpha = 1$, and $\alpha = 0.5$, were considered. As shown in Fig. 2, the agreement between the theoretically determined pdf and the pdf estimated from each of these simulations is excellent.

One may ask how this result differs from a naive application of an implicit scheme as follows:

$$x_1(t_{n+2}) = x(t_n) + 2a_1(t_{n+1}, x(t_{n+1}))\Delta, \qquad (14a)$$

$$x(t_{n+2}) = x_1(t_{n+2}) + 2a_2(t_{n+2}, x(t_{n+2}))\Delta, \qquad (14b)$$

where, now,

$$a_2 = [k^2 - (r_o + r_s\eta)]x, \qquad (14c)$$

and where η is a Gaussian random number with zero mean and unit variance. The initial condition, time step, spinup time, etc., are all chosen to be the same as in the experiment with ET03b. The pdf resulting from this integration (Fig. 2) is highly peaked around the deterministic steady state at $x_d = 1$ rather than at the true peak at $x_p = 0.862$, an error of 16%. More severe are a large underestimation of the standard deviation, which is about an order of magnitude too small, and an overestimation of the maximum probability density, which is a factor of about 8.7 too large. Naive use of Runge–Kutta schemes, either of order two or of order four, yields similar results (not shown).

5. Example 3: Application to El Niño

There are two basic approaches to developing a stochastic numerical model of El Niño: forward modeling and inverse modeling. In the forward modeling approach, one takes the primitive equations of the ocean (Lions et al. 1992) or, better, the coupled equations of the ocean–atmosphere system (Lions et al. 1993, 1995) and applies a systematic scaling theory (the CLT) as proposed by Majda et al. (1999). The alternative approach, which is what we adopt here, is to assume a basic dynamical form for the propagation equations, estimate those equations from data, and then use dynamical restrictions on the observed statistics to verify whether or not the basic dynamical assumptions hold. This was the approach taken by Penland and Magorian (1993), Penland and Sardeshmukh (1995), and others, who assumed a simple stable, linear process driven by additive white noise as their model of tropical Indo-Pacific SSTs. They tested their assumptions with a rather stringent statistical criterion called the ‘‘tau test,’’ which was shown to be consistent with the observations.

Any model of tropical Indo-Pacific SST should reproduce the contemporaneous and lagged statistics of the observations. At issue is whether the skew toward warm SST observed in most El Niño indices precludes the stochastic model (LIM) of El Niño advanced by Penland and Sardeshmukh (1995). As in previous studies, we consider tropical Indo-Pacific sea surface temperatures in the area 30°N–30°S, 30°E–70°W from the Comprehensive Ocean–Atmosphere Data Set (COADS; Woodruff et al. 1993). In agreement with our current forecasting method (Penland et al. 2003), we consolidate these data onto a 4° × 10° grid, subject them to a 3-month running mean, remove the 1950–2000 climatological annual cycle, and project them onto the leading 17 EOFs containing approximately two-thirds of the variance. The leading EOF of these data is dominated by a classic El Niño pattern (not shown; see references cited above), and the corresponding coefficient time series [principal component (PC)] explains 26% of the SST anomaly variance. What we shall do here is compare the statistics of a system with only additive noise to systems with multiplicative noise to see if the data support the more complicated assumptions.

Using COADS data between January–February–March 1950 and October–November–December 2000 (i.e., 598 maps) processed as discussed above, a Green function $\mathbf{g}(\tau_o)$ is evaluated at a representative lead time of $\tau_o = 4$ months:

$$\mathbf{g}(\tau_o) = \mathbf{C}(\tau_o)\mathbf{C}^{-1}(0), \qquad (15)$$

where $\mathbf{C}(\tau)$ is the covariance matrix of the SST anomalies at lead time τ. In previous work, this Green function has been associated with the matrix $\exp(\mathbf{L}\tau_o)$, where it has been assumed that the SST anomalies $\delta\mathbf{T}$ obey the Langevin equation

$$d\delta\mathbf{T} = \mathbf{L}\,\delta\mathbf{T}\,dt + \mathbf{S}\,d\mathbf{W}. \qquad (16)$$

We call $\mathbf{g}(\tau_o)$ a Green function since, for the system described by Eq. (16), the most probable prediction of $\delta\mathbf{T}(\tau)$ at lead time τ given an initial condition $\delta\mathbf{T}(0)$ is $\mathbf{g}(\tau)\,\delta\mathbf{T}(0)$. Obviously, one need not recalculate the SST covariance structure for any τ different from τ_o to make a prediction; rather one exploits the eigenstructure of $\mathbf{g}(\tau_o)$ to estimate $\mathbf{L}$ and, thus, $\mathbf{g}(\tau)$ (Penland 1989). With a data-derived estimate for $\mathbf{L}$, one estimates the matrix $\mathbf{SS}^T$ from the appropriate fluctuation–dissipation relation (FDR) as follows:

$$\mathbf{LC}(0) + \mathbf{C}(0)\mathbf{L}^T + \mathbf{SS}^T = 0. \tag{17}$$

Note that the matrix $\mathbf{S}$ can be diagnosed from Eq. (17) only up to an arbitrary unitary matrix; however, any of these nonunique matrices $\mathbf{S}$ employed in a numerical model will provide the observed contemporaneous and lagged covariance statistics of $\delta\mathbf{T}$.

If we confine ourselves to considering predictions most accurate in the least squares sense, there is an alternative interpretation to $\mathbf{g}(\tau)$. If $\delta\mathbf{T}$ obeys a Stratonovich multiplicative Langevin equation

$$d\delta\mathbf{T} = \mathbf{L}\delta\mathbf{T}dt + \mathbf{A}\delta\mathbf{T}dW_1 + \mathbf{S}d\mathbf{W}_2 \tag{18}$$

rather than Eq. (16), then we may interpret the Green function as $\exp([\mathbf{L} + 0.5\mathbf{A}^2]\tau_o)$ (e.g., Sardeshmukh et al. 2001a). The corresponding FDR for this system is evaluated by taking second moments of the Fokker–Planck equation (e.g., Penland and Matrosova 1994):

$$(\mathbf{L} + 0.5\mathbf{A}^2)\mathbf{C}(0) + \mathbf{C}(0)(\mathbf{L} + 0.5\mathbf{A}^2)^T + \mathbf{SS}^T + \mathbf{AC}(0)\mathbf{A}^T = 0. \tag{19}$$

Now, one may estimate the combination $(\mathbf{L} + 0.5\mathbf{A}^2)$ from data [Eq. (15)], and, hence, the combination $[\mathbf{SS}^T + \mathbf{AC}(0)\mathbf{A}^T]$ from Eq. (19). However, it is possible to isolate $\mathbf{A}$ only in special cases. Thus, we choose two reasonable but arbitrary models for $\mathbf{A}$. First, since at small lead times the covariance of the prediction error is proportional to $[\mathbf{SS}^T + \mathbf{AC}(0)\mathbf{A}^T]$ [Eq. (19); appendix A of Penland and Matrosova (1994)], we estimate $\mathbf{A}$ by regressing the $\tau = 1$ month prediction error incurred during the training period onto the verification. Note that we are not trying to judge the prediction skill of the model; we are still trying to obtain best estimates of parameters. We then subtract $\mathbf{A}^2/2$ from the matrix logarithm of the Green function to estimate the deterministic feedback matrix $\mathbf{L}$. The additive noise matrix $\mathbf{SS}^T$ is diagnosed from the residual of the FDR [Eq. (19)]. We call this multiplicative model 1 (MM1).

Our second model of $\mathbf{A}$ assumes that the multiplicative noise comes from random components in the damping. That is, if β_α is the α th eigenvalue of $\mathbf{L}$, and $\mathbf{u}_\alpha$, $\mathbf{v}_\alpha$ are its corresponding eigenvector and adjoint, respectively, we assume Eq. (18) has the form

$$d\delta\mathbf{T} = \mathbf{L}\delta\mathbf{T}dt + \mathbf{u}(\mathbf{Re}\boldsymbol{\beta})\mathbf{v}^T\delta\mathbf{T}dW_1 + \mathbf{S}d\mathbf{W}_2. \tag{20}$$

In Eq. (20), $\mathbf{u}$ is the matrix, the α th column of which is an eigenvector $\mathbf{u}_\alpha$ of $\mathbf{L}$; $\mathbf{v}$ is the corresponding matrix of adjoints; and $\mathbf{Re}\ \boldsymbol{\beta}$ is the diagonal matrix, the α th diagonal element of which is $\mathrm{Re}(\beta_\alpha)$ of $\mathbf{L}$. Note that this diagonal matrix is negative definite, hence, its identification with the damping. In this case $\mathbf{A}$ and $\mathbf{L}$ are estimated simultaneously from the data and, again, the additive noise matrix is diagnosed from the residual of the FDR. This is multiplicative model 2 (MM2).

We first integrated Eq. (18) for 48 000 ''months'' using a time step of 1/(60 months) and using parameters described in Penland et al. (2003). All numerical calculations were performed in the 17-dimensional EOF space. Initial conditions were chosen at the peak of the marginal distribution at $\delta\mathbf{T} = 0$ and the model was spun up for 1000 months. For this problem, differences in sample paths resulting from integrations using the implicit and explicit schemes were found to be negligible. The two schemes yielded results similar to each other in the multiplicative noise case as well.

The long time series was divided into 80 ensemble members, each having a length of 600 months. This number of ensemble members was chosen since it is about the same size as ensembles used when investigating the statistics of general circulation models (e.g., Compo et al. 2001). The same procedure was then applied to MM1 and MM2. By construction, each model should reproduce the observed mean and covariance structure, and this was verified from the model output. The sample skew, kurtosis, and trend of the leading numerically generated PC (PC1) were then evaluated for each ensemble of each model. Histograms of the resulting sample statistics are compared in Figs. 3–5, with sample statistics from the observed PC1 indicated by vertical lines on the graphs.

It is seen in Fig. 3 that the effect of the multiplicative noise in both cases is to increase the values of skew available to finite samples over what might be expected when the noise is additive. Although the histograms are roughly centered at 0 as they ought to be, the distribution of sample skew is clearly narrower when the noise is additive than it is in either of the multiplicative noise cases. The sample skew of the observed PC1 (0.28) fits comfortably within the distribution of sample skew for any of the three stochastic models.

A similar story is told by the statistics of sample kurtosis (Fig. 4); the values of kurtosis available to finite samples from the multiplicative noise models is greatly increased over those available to the additive noise model. Again, the sample kurtosis of the observed PC1 (0.14) fits comfortably within the distribution of sample kurtosis for any of the three models. However, the true kurtosis of the multiplicative noise models need not be 0 since these models allow large excursions away from the mean $\langle\delta\mathbf{T}\rangle = 0$, and that appears to be the case for MM2 in particular. Further, the distributions of sample kurtosis for both of these multiplicative noise models have a significant positive skew.

Figure 5 suggests that the type of noise does not play much of a role in the shape of the distribution of sample trends for the modeled PC1. It *is* interesting that reproducing the sample trend in the observed PC1 (0.12° yr^{-1}) is unlikely in all three models. In the additive noise model, only 7 of 80 cases have a trend with ab-

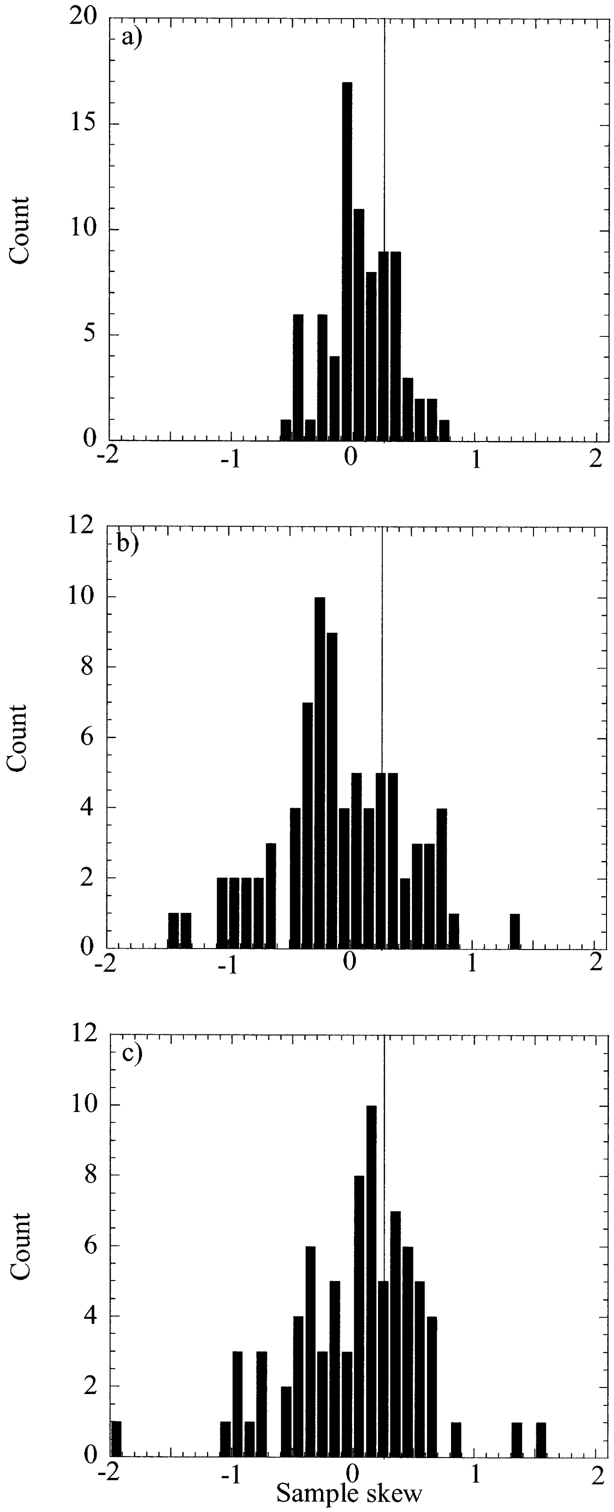

FIG. 3. Histogram of sample skew estimated from 80 members of an ensemble generated by a numerical stochastic model of El Niño: (top) additive noise model; (center) MM1, and (bottom) MM2.

solute value greater than 0.12° yr^{-1}, so that by this measure the observed trend in PC1 is significant at about the 9% level. This result corroborates work performed with D. Sun and T. Zhang (2003, personal communication).

6. Discussion

Many of the most divisive issues in the scientific community involve disagreements about which dynamical regimes constitute a correct description of various geophysical systems, and most of the arguments are based on numerical simulations. The issue concerning the dynamical nature of El Niño has received a particularly large amount of attention; realistic-looking El Niño–like behavior has been found in numerical models with fixed-point (e.g., Moore and Kleeman 1997a,b; Penland and Matrosova 1994; Thompson et al. 2000; Penland et al. 2000), limit-cycle (e.g., Schopf and Suarez 1988, 1990; Battisti 1988; Battisti and Hirst 1989; Barnett et al. 1993; Syu et al. 1995; Blanke et al. 1997), or chaotic (e.g., Münnich et al. 1991; Jin et al. 1994; Tziperman et al. 1994) attractors. Given the irregular nature of El Niño, some sort of stochastic forcing appears necessary in the fixed-point and limit-cycle scenarios and, in varying degrees of rigor, has already been implemented in some numerical models of El Niño. As we in this study and others (e.g., Sura and Penland 2002) have shown, the choice of integration technique can greatly affect the outcome of a stochastically forced numerical model, and the variety of results possible in different implementations of a single conceptual model is frightening.

Another important issue in geophysics is whether the atmospheric circulation supports distinct weather regimes due to nonlinear dynamics (e.g., Charney and DeVore 1979; Legras and Ghil 1985; Corti et al. 1999) or whether the atmosphere is basically a linear dynamical system supported by stochastic forcing (e.g., Farrell 1985, 1988; DelSole and Hou 1999; Whitaker and Sardeshmukh 1998). Again, numerical results are likely to depend crucially on the choice of stochastic integration techniques.

Some may claim that the choice of integration algorithm is not as important if the stochastic forcing is additive, or if the stochastic forcing is red rather than white. Even if the dynamical system is an additive noise process, the stochastic forcing may still affect the mean dynamics of a multivariate nonlinear system. Indeed, this was the case in the numerical study by Sura and Penland (2002). The effect of multiplicative *red* (rather than white) noise on even a linear system can also be important. For example, the analytical study by Sardeshmukh et al. (2001b) showed how red fluctuations in the damping coefficient of a linearized barotropic vorticity model caused the mean stationary state to have a magnitude larger than the stationary state of the cor-

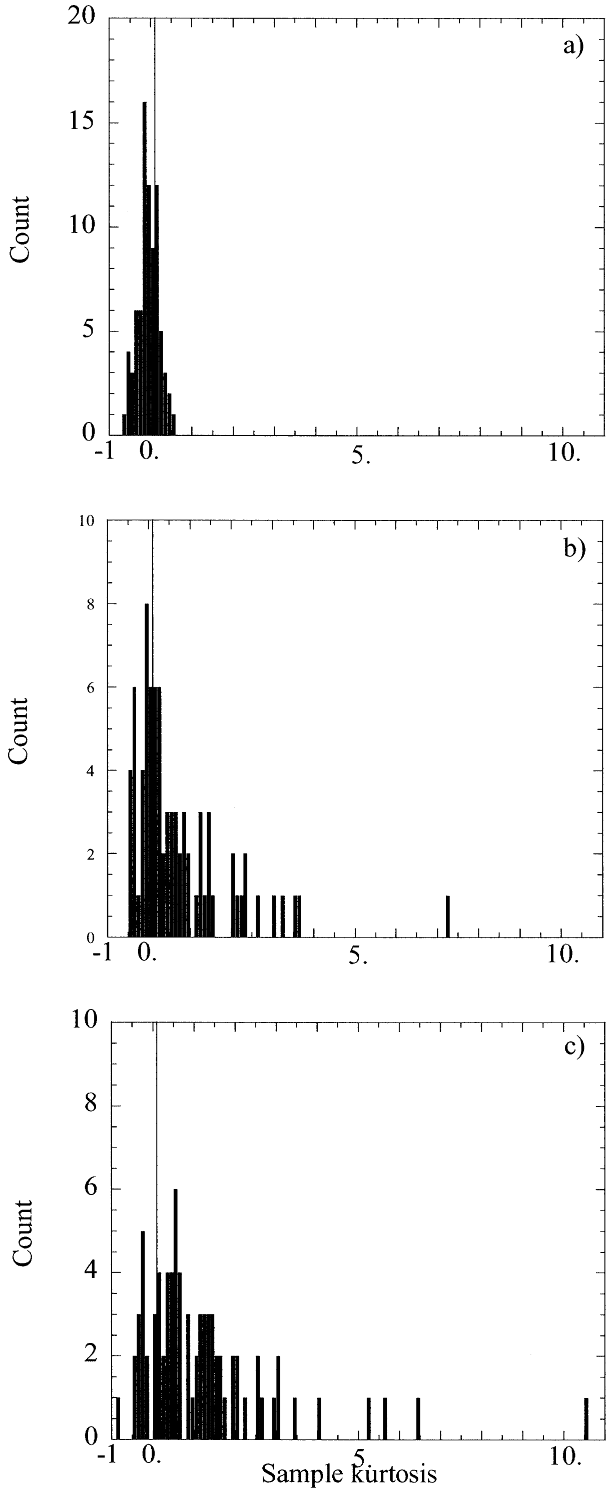

FIG. 4. As in Fig. 3, but for the sample kurtosis.

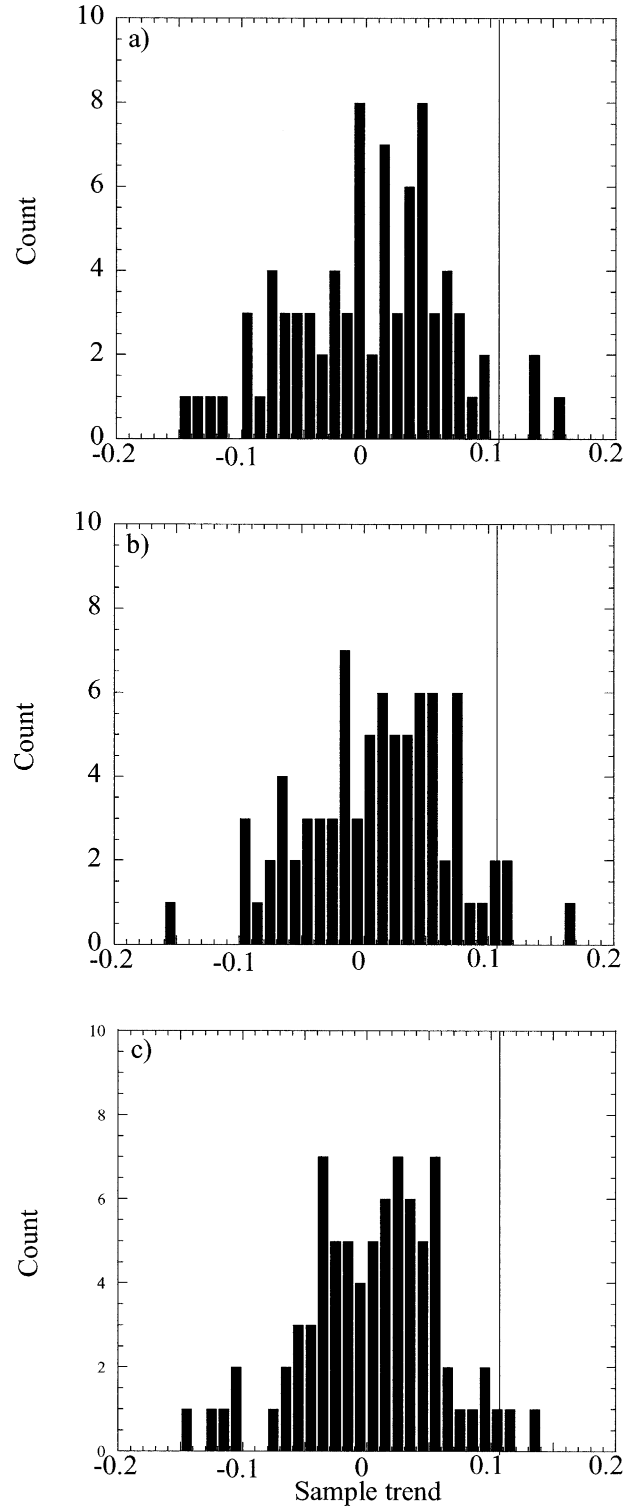

FIG. 5. As in Fig. 3, but for the sample trend.

responding deterministic model. In contrast, red fluctuations in the background zonal velocity tended to damp the mean state, but with a pattern that could not completely cancel the effects of a stochastic damping. In fact, the two results are related: white noise forcing added to one component of a multivariate dynamical system translates into multiplicative red noise forcing of another component if the two components are related nonlinearly. We repeat: numerical results are likely to be corrupted by improper integration techniques.

In this work, we do not merely demonstrate the existence of a dangerous situation, but also offer methods for ameliorating it. These methods have been developed with the architecture of current atmospheric models in mind so that prohibitively extensive revision of those models may be avoided. Both explicit and implicit schemes have been presented and illustrated with simple examples. Further, we have compared these schemes with commonly used alternatives and shown how severe the errors obtained with naive implementations can be.

It is natural to ask what advantages ET03 schemes might have over earlier stochastic integration schemes such as Heun and Mil'shtein. We have demonstrated the superior convergence properties of ET03a compared to Heun in our example with the genic models. Advantages over Mil'shtein schemes are situation dependent. In particular, the Mil'shtein schemes require much more computation if the system satisfies a complicated evolution equation, particularly if that system is high dimensional. The difference in computational effort is due to the fact that Mil'shtein schemes generally require at least twice as many evaluations of the evolution equation than do the ET03 schemes. There is an exception: if the multiplicative noise enters the evolution equations in a linear manner, then ET03a turns out to be equivalent to one of the Mil'shtein schemes. The ET03b scheme, in contrast, differs from the Mil'shtein schemes in that ET03b supports a division of the deterministic contribution to the tendency into an explicit part as well as an implicit part. The extension can be crucial if the entire updating operator cannot be inverted. That would have been the case in our El Niño model had we been obliged to run a modified version of our EOF-filtered model in geographical space. Finally, unlike Mil'shtein schemes, the ET03b scheme allows a leapfrog step, thus obviating the need to rewrite a large part of many existing climate models.

Both ET03 schemes yielded similar results when applied to additive and multiplicative noise models of tropical Indo-Pacific SST. The models do not support the need to assume multiplicative noise in a stochastic model of El Niño, nor do they support a significant asymmetry between warm and cold events as has been sometimes claimed in the literature (e.g., see the online discussion at http://www.ecmwf.int/products/forecasts/seasonal/documentation/ch3.html). However, according to both additive and multiplicative stochastic models of El Niño, the observed trend in the leading principal component of tropical Indo-Pacific SST anomalies during the last 50 years is unlikely to be explained by sampling. The possibility that deterministic external forcing may be causing this trend is unavoidable, and further work is clearly needed.

In spite of the fact that Hasselmann's (1976) paper appeared more than a quarter of a century ago, these are still the early days of stochastic modeling in the atmospheric sciences. In some part, that is because the basic science of stochastic processes is still largely unexplored, especially how to exploit those processes' ability to represent deterministic, high-dimensional chaotic systems in a dynamically consistent manner. The scientist's need for numerical methods for treating highly complex systems consisting of important interactions between physical phenomena with widely different time scales can offer the applied mathematician a rich variety of unsolved problems. It is possible that the needs of climate research may even play a role in guiding the development of stochastic numerical analysis as a mature academic discipline, to the obvious advantage of both disciplines.

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