Nonequilibrium Statistical Mechanics of Tropical Sea Surface Temperature Variability

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Climate variability has significant human impact but is difficult to model and predict. Recent theoretical developments in nonequilibrium statistical mechanics cover a class of stochastic models often used for climate phenomena. The theory for a coarse-grained entropy production is developed for simple stochastic climate models and applied to observed tropical sea surface temperatures (SST), demonstrating that nonequilibrium properties can be quantified with climate datasets, and that tropical SST variability is approximately consistent with fluctuations about a nonequilibrium steady-state with relatively few degrees-of-freedom. Fluctuations with negative entropy production demonstrate that seasonal tropical SST variability is small and fast in a thermodynamic sense, indicating that nonequilibrium fluctuation theory is applicable. This work demonstrates that nonequilibrium theory can address climate-scale phenomena, suggests that it could provide insight into how climate change will affect climate variability, and perhaps provide a fundamental theory for variability of the climate system.

1. Introduction

The climate system self-organizes into many distinct recognizable features such as El-Niño, the Atlantic Gulf Stream, and the mid-latitude storm tracks. While the mean state of these features is reasonably well captured by complex coupled global climate models, their variability is typically more difficult to capture in models, is poorly understood from a theoretical perspective, and yet has large human impacts [*Solomon et al.*, 2007; *Min et al.*, 2005; *Zhang and McPhaden*, 2006; *Wunsch*, 2008; *van Oldenborgh et al.*, 2005; *Collins*, 2005; *Spencer et al.*, 2005; *Greeves et al.*, 2007; *Ulbrich*, 2008]. Simple stochastic climate models provide predictions of some climate phenomena that are on par with detailed dynamical models [*Newman et al.*, 2003; *Saha et al.*, 2006]. Recently, it has become clear that these models implicitly assume that the variability of climate features is a manifestation of fluctuations about a nonequilibrium steady-state [*Weiss*, 2007]. This leads one to consider the application of the statistical mechanics of nonequilibrium systems to climate variability. Here we consider nonequilibrium steady states in the context of simple stochastic climate models but note that the concept is applicable to more complex models as well.

Recent breakthroughs in statistical mechanics in the form of fluctuation theorems have revolutionized our understanding of nonequilibrium systems [*Evans et al.*, 1993; *Gallavotti and Cohen*, 1995; *Evans and Searles*, 2002; *Sevick et al.*, 2008]. Previous work on fluctuation theorems has focused on micro-scale systems such as RNA molecules and molecular machines [*Sevick et al.*, 2008]. Fluctuation theorems quantify the likelihood of finding fluctuations that decrease entropy. In accordance with the Second Law of Thermodynamics, these fluctuations are exponentially unlikely in large systems at long times. But for small systems at short times, such "backwards" fluctuations are observable [*Evans and Searles*, 2002; *Sevick et al.*, 2008]. This requirement of small scales would seem to preclude the application of fluctuation theory to climate phenomena. However some climate features may be dynamically small in terms of their degrees-of-freedom and fast in terms of the relevant timescales, and thus could potentially exhibit entropy reducing fluctuations.

2. Stochastic Climate Models

Simple stochastic climate models have long been used to study the climate system [*Epstein*, 1969; *North and Cahalan*, 1981; *Penland and Magorian*, 1993; *Penland and Sardeshmukhn*, 1995; *Farrell and Ioannou*, 1993; *Moore and Farrell*, 1993]. In the simplest models, sometimes called Langevin models, the state of the system is described by a real N dimensional vector $\mathbf{x}$, the linear dynamics and noise amplitude are described by real $N \times N$ matrices $\mathbf{A}$ and $\mathbf{F}$, the diffusion matrix is $\mathbf{D} = \mathbf{F}\mathbf{F}^T/2$, superscript T denotes the matrix transpose, ξ is N dimensional Gaussian white noise, and the dynamics is given by

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x} + \mathbf{F}\xi. \tag{1}$$

Langevin systems have been used to study climate features including El-Niño [*Penland and Magorian*, 1993], the Gulf Stream [*Moore and Farrell*, 1993], and mid-latitude storm tracks [*Newman et al.*, 2003]. In the case of tropical sea surface temperature (SST) the deterministic part represents slowly evolving ocean dynamics and the random noise represents the fast chaotic atmosphere at timescales beyond the Lyapunov predictability limit.

Langevin models such as equation (1) are among the simplest mathematical models of a nonequilibrium steady-state. Linear stochastic systems can have surprisingly complex and ordered behavior arising from matrix non-commutivity rather than nonlinearity. When $\mathbf{AD} \neq \mathbf{DA}^T$, equation (1) describes a nonequilibrium system where small noise is amplified into large finite-time events with well-defined lifecycles [*Ioannou*, 1995; *Weiss*, 2003]. These models display the essential features of nonequilibrium fluctuations and are simple enough that quantitative calculations can be performed and compared with observations.

Linear inverse models are models where the governing matrices in equation (1) , $\mathbf{A}$ and $\mathbf{F}$, are obtained by fitting to observed data. Here we use the linear inverse model for tropical SST of *Penland and Matrosova* [2006]. In this model, the Comprehensive Ocean-Atmosphere Data Set (COADS)

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[*Woodruff et al.*, 1993] of monthly SST in the tropical strip from 30° S to 30° N from 1950-2000 was consolidated onto a 4° × 10° grid, subjected to a three-month running mean, and the 1950-2000 climatology was removed. The resulting data was then projected onto the first 20 empirical orthogonal functions, which were used to construct $\mathbf{A}$, and $\mathbf{F}$, providing a 20-dimensional empirical stochastic model for seasonal SST dynamics. While this model has been shown to have skill for seasonal SST predictions, its thermodynamic properties have not been previously investigated.

3. Entropy Production

Non-equilibrium steady-states are maintained away from equilibrium by the production of entropy. Here we study thermodynamic concepts of nonequilibrium entropy production, in contrast to previous work on information theoretic concepts of entropy [*DelSole and Tippett*, 2007]. For a system in a nonequilibrium steady-state, a finite trajectory segment has an entropy production σ given by the ratio of the probabilities of finding the trajectory segment and its time-reversed counterpart [*Seifert*, 2005]:

$$\sigma = \ln \frac{P[\mathbf{X}]}{P[\hat{\mathbf{X}}]}, \tag{2}$$

where $\mathbf{X}$ is a trajectory segment from t to $t+\tau$, $\mathbf{X} = \{\mathbf{x}(t+s)\}_{s=0}^{\tau}$, $\hat{\mathbf{X}}$ is the time-reversed trajectory $\hat{\mathbf{X}} = \{\mathbf{x}(t+\tau-s)\}_{s=0}^{\tau}$, $P[\mathbf{X}]$ is the probability of finding path $\mathbf{X}$ in the steady-state, and $P[\hat{\mathbf{X}}]$ is the probability of finding the time-reversed path in the steady-state.

When data is finitely sampled, the continuous trajectory is not available and one must turn to a coarse-grained entropy production. Coarse-grained entropy productions are always less than or equal to the total entropy production, and have been used to provide a lower bound on the dissipated work [*Gomez-Marin et al.*, 2008]. One specific coarse-graining is to consider only the dependence on the endpoints of the trajectory segment, which we call the endpoint entropy production σ_e, obtained from considering all trajectories with timespan τ with fixed initial and final endpoints, $\mathbf{x_0}$ and $\mathbf{x_1}$. The full path probability can be written in terms of the coarse-grained probability of finding a trajectory segment with endpoints $\mathbf{x}(t) = \mathbf{x}_0$ and $\mathbf{x}(t+\tau) = \mathbf{x}_1$ regardless of the intervening path, $P[\mathbf{x}_0, \mathbf{x}_1]$, and the conditional probability of finding the path $\mathbf{X}$ with the given endpoints, $P[\mathbf{X}|\mathbf{x}_0, \mathbf{x}_1]$:

$$P[\mathbf{X}] = P[\mathbf{X}|\mathbf{x}_0, \mathbf{x}_1]P[\mathbf{x}_0, \mathbf{x}_1]. \tag{3}$$

One obtains σ_e as the analog of the total entropy production but calculated from the coarse-grained probability distribution function (pdf)

$$\sigma_e = \ln \frac{P[\mathbf{x}_0, \mathbf{x}_1]}{P[\hat{\mathbf{x}}_0, \hat{\mathbf{x}}_1]}, \tag{4}$$

where $\hat{\mathbf{x}}_0 = \mathbf{x}_1$ and $\hat{\mathbf{x}}_1 = \mathbf{x}_0$.

Define the average over trajectories with fixed endpoints to be

$$\langle F \rangle_e = \int_{\substack{\mathbf{x}(t)=\mathbf{x}_0 \\ \mathbf{x}(t+\tau)=\mathbf{x}_1}} \mathcal{D}\mathbf{x}(s)\, P[\mathbf{X}|\mathbf{x}_0, \mathbf{x}_1]\, F. \tag{5}$$

It is then straightforward to show that the total and coarse-grained entropy productions σ and σ_e are related by

$$\left\langle e^{-\sigma} \right\rangle_e = e^{-\sigma_e}. \tag{6}$$

Thus, if σ_e is negative, this implies that there exist trajectory segments with negative total entropy production, and further, that there are enough of them for the average in equation (6) to be greater than one.

Recently a theory was developed for systems described by equation (1) relating the statistics of σ_e to the governing matrices $\mathbf{A}$ and $\mathbf{F}$ [*Weiss*, 2007]. In this previous work the quantity here called σ_e was not recognized as a coarse-grained entropy and the above connection to the total entropy production was not established. The theory does show that σ_e satisfies a fluctuation theorem: trajectory segments with positive σ_e are exponentially more likely than those with negative σ_e, $p_\tau(\sigma_e)/p_\tau(-\sigma_e) = \exp(\sigma_e)$, where the pdf $p_\tau(\sigma_e)$ is the probability that a trajectory segment has entropy production σ_e.

We now state the results of this previous theory which we will here apply to tropical SST observations. Define the finite time $N \times N$ dimensional covariance matrix

$$\mathbf{C}_\tau = 2\int_{-\tau}^{0} ds\, e^{-\mathbf{A}s}\mathbf{D}e^{-\mathbf{A}^T s}, \tag{7}$$

the steady-state covariance $\mathbf{C}_0 = \lim_{\tau\to\infty} \mathbf{C}_\tau$, and their inverses $\mathbf{Q}_\tau = \mathbf{C}_\tau^{-1}$, $\mathbf{Q}_0 = \mathbf{C}_0^{-1}$. Define the $2N \times 2N$ dimensional block-matrices $\mathbf{R}_{01}$, $\mathbf{R}_{10}$, and $\mathbf{R}$,

$$\begin{aligned}
\mathbf{R}_{01} &= \begin{pmatrix} e^{\mathbf{A}^T\tau}\mathbf{Q}_\tau e^{\mathbf{A}\tau} + \mathbf{Q}_0 & -e^{\mathbf{A}^T\tau}\mathbf{Q}_\tau \\ -\mathbf{Q}_\tau e^{\mathbf{A}\tau} & \mathbf{Q}_\tau \end{pmatrix}, \\
\mathbf{R}_{10} &= \begin{pmatrix} \mathbf{Q}_\tau & -\mathbf{Q}_\tau e^{\mathbf{A}\tau} \\ -e^{\mathbf{A}^T\tau}\mathbf{Q}_\tau & e^{\mathbf{A}^T\tau}\mathbf{Q}_\tau e^{\mathbf{A}\tau} + \mathbf{Q}_0 \end{pmatrix},
\end{aligned} \tag{8}$$

$\mathbf{R} = \mathbf{R}_{10} - \mathbf{R}_{01}$, and the $2N$ dimensional endpoint vector $\mathbf{z} = (\mathbf{x}_0, \mathbf{x}_1)$. Then for a given trajectory segment, the endpoint entropy production is

$$\sigma_e(\mathbf{x}_0, \mathbf{x}_1) = \frac{1}{2}\mathbf{z}^T\mathbf{R}\mathbf{z}. \tag{9}$$

The theory gives $p_\tau(\sigma_e)$ and its moments in terms of the governing matrices. Define a matrix $\mathbf{W} = \mathbf{R}_{01}^{-1}\mathbf{R}$. Then the mean and variance are given by [*Weiss*, 2007, equation 25]

$$\langle\sigma_e\rangle = \mathrm{Tr}(\mathbf{W})/2, \qquad \left\langle(\sigma_e - \langle\sigma_e\rangle)^2\right\rangle = \mathrm{Tr}(\mathbf{W}^2)/2, \tag{10}$$

where the average is over all endpoints. The characteristic function of $p_\tau(\sigma_e)$ is [*Weiss*, 2007, equation 21]

$$\hat{p}_\tau(k) = \frac{1}{\prod_{n=1}^{2N}\sqrt{1 - ik\lambda_n}}, \tag{11}$$

where λ_n are the eigenvalues of $\mathbf{W}$, and $p_\tau(\sigma_e)$ is obtained from its characteristic function by the usual relationship.

4. Entropy production of tropical SST

We investigate whether the entropy production of fluctuations in tropical SST match the predictions made by assuming that the system is in a nonequilibrium steady-state governed by equation (1). We thus look at $p_\tau(\sigma_e)$ and its dependence on the segment time τ. A direct test of the fluctuation theorem is not feasible due to the relatively short 50 year SST time series.

The pdf and its moments can be calculated by two separate methods. They can be calculated from equations (10) and (11), which we refer to as the theoretical method. Alternatively, for each trajectory segment one can obtain σ_e directly using equation (9). These individual entropy productions can be used to directly compute moments and compiled into a pdf, which we refer to as the direct method. For a system that is exactly described by equation (1), the methods must agree, apart from sampling errors due to using a finite number of trajectory segments in the direct method. But if the system is not governed by Langevin dynamics, then there is no reason to expect the methods to agree. Since both methods use the same governing matrices, which are themselves derived from the timeseries used in the direct method, they are not independent. Agreement between the two methods thus demonstrates the self-consistency of Langevin dynamics, and indicates that the variability is consistent with fluctuations about a linear nonequilibrium steady-state. The coarse-grained entropy production provides a new test for the validity of Langevin dynamics which is independent from the tau-test used by *Penland and Sardeshmukhn* [1995].

Using the linear inverse model of *Penland and Matrosova* [2006] we calculate the average, variance, and pdf of σ_e. The average over all endpoints, $\langle\sigma_e\rangle(\tau)$, has a broad maximum at three to five months and decays to near zero over two years (Figure 1a). This is consistent with the known timescales for El-Niño events. The error-bars indicate the standard error in the direct calculation due to finite sample size, assuming that the governing matrices are exact and the segments are independent. These assumptions imply that the true uncertainty in the comparison is larger than indicated by the error bars. For times longer than the three-month averaging time of the data, the average from the two methods agrees extremely well, while for shorter times we do not expect the Langevin model to be accurate. The variance of σ_e shows qualitative agreement between the two methods, but the differences are larger than the lower bound indicated by the error bars (Figure 1b).

The pdf's calculated by the two methods have the same general shape and similar evolution with τ (Figure 2). They have long tails for positive σ_e, finite probability of negative σ_e, and as the segment time increases they become narrower and the peak decreases towards zero. The trajectory segments with negative σ_e imply that there exist "backwards" trajectories with negative total entropy production. Thus, on timescales of months, the seasonally averaged tropical SST can be considered a small, fast system in thermodynamic terms where "violations" of the Second Law of Thermodynamics are likely to occur, albeit with a small probability.

The entropy production which maintains the nonequilibrium steady-state results in a long-term average rate of entropy production in the thermal reservoir producing the noise. Here, the reservoir is the chaotic atmosphere whose time-average entropy production rate is bounded by the sum of its positive Lyapunov exponents [*Eckmann and Ruelle*, 1985]. The average rate of this entropy production can be calculated from the governing matrices [*Weiss*, 2007, equation 33] and its inverse gives a time of 3.6 days, which roughly agrees with the Lyapunov predictability time of the atmosphere. Thus, even in a white-noise model which assumes that the timescale of the atmospheric forcing is so small as to be effectively zero, the slow seasonally averaged SST dynamics retains information about the finite predictability time of the fast chaotic atmosphere.

5. Conclusions

The entropy production statistics show that tropical SST dynamics on seasonal timescales is approximately self-consistent with a simple nonequilibrium Langevin model, and thus that tropical SST variability can be considered to be a manifestation of fluctuations about a nonequilibrium steady-state. This is perhaps not surprising, since the ocean is clearly not in equilibrium and it is not uncommon to treat natural variability in terms of a stationary state. However, the fact that a relatively simple Langevin model with few degrees of freedom correctly captures the entropy production indicates that SST variability can be studied using quantitative theories of nonequilibrium statistical mechanics which provide new insight into the detailed behavior of such nonequilibrium fluctuations. The presence of SST fluctuations with negative entropy production indicates that SST variability is in the regime of small, fast thermodynamic fluctuations. This work also demonstrates that typical climate datasets are sufficient to calculate the nonequilibrium thermodynamic properties of the climate system.

The construction of the linear inverse model has a small number of subjective choices, but the model was defined for other purposes, used with here with no modifications, and the computations presented here have no free parameters. The ability of the model to capture the entropy production shows that, in addition to its utility as a forecast model, it is robust enough to be used for thermodynamic purposes. The Langevin model is only approximate as demonstrated by the discrepancies between the two methods, particularly in the entropy production variance. But the concept of climate variability as fluctuations about a nonequilibrium steady-state is much broader than the simple linear model studied here.

Theories of nonequilibrium fluctuations have the potential of providing, for the first time, a fundamental quantitative theory for natural climate variability. Further development of the theory to include processes such as nonlinearity, colored and multiplicative noise, and the seasonal cycle should lead to additional improvements. Given the simplicity of the linear model, particularly compared to a full coupled general circulation model, the success is striking.

Since simple Langevin models are useful for a range of climate phenomena, we expect that other climate features will also prove to be at least approximately represented as fluctuations about a nonequilibrium steady-state. For example, considering the SST and thermocline depth as state variables would provide a theory for natural variability in upper-ocean heat content which has been the topic of much recent interest (e.g., *Carton and Santorelli* [2008]). Applying these ideas to energy balance climate models (e.g., *North and Cahalan* [1981]) could result in a theory for the natural variability of poleward heat flux. By expanding the theory to include adiabatic changes in the governing matrices, the influence of climate change on El-Niño variability could be addressed.

We must mention that the word "steady" in the conclusion that tropical SST can be represented by a nonequilibrium steady-state in no way contradicts the ocean warming observed over the past fifty years [*Levitus et al.*, 2005]. The seasonal SST variability is much larger than the warming of the average state and changes in the governing matrices due to this warming are too small to be reliably estimated from a 50-year dataset. Yet the steady-state is changing and the impact of these changes on the variability is important in predicting the impacts of global warming. The relevance of nonequilibrium steady-states demonstrated here indicates that recent and future advances in nonequilibrium statistical mechanics may play a role in improving forecasts of global change.

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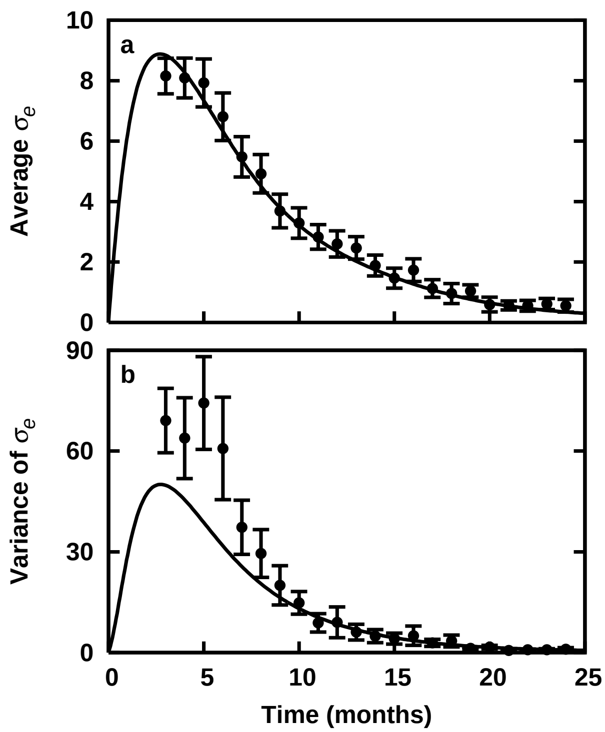

Figure 1. Average and variance of the endpoint entropy production as a function of trajectory segment time. Solid line denotes the theoretical method, and filled circles denote the direct method. The error bars show the standard error based on the number of trajectory segments of a given segment time in the 50 year dataset. Panel a shows the average, and panel b shows the variance.

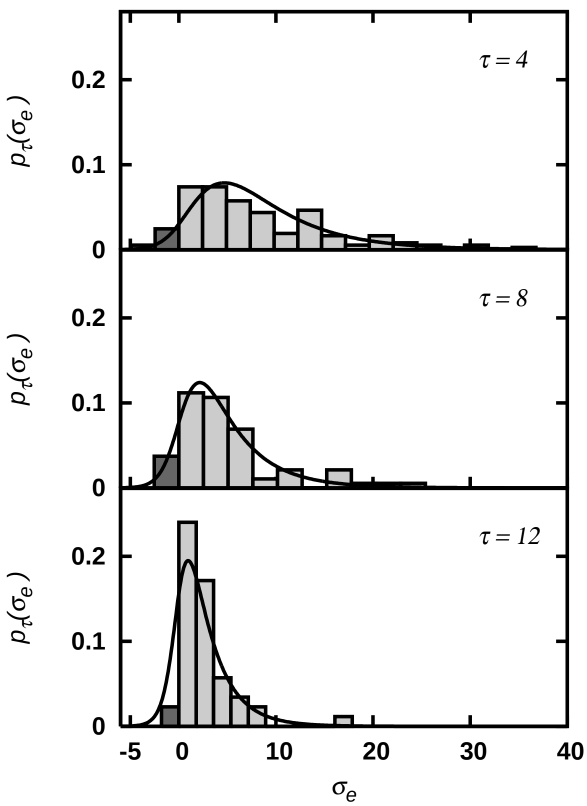

Figure 2. Probability distribution function of the end-point entropy production. The solid curve is the distribution from the theoretical method and the binned distribution is calculated using the direct method. The darker shaded bins show trajectory segments with negative entropy production.